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AN IMPLICIT, WIGGLE-FREE, AND ACCURATE UPSTREAM FINITE-DIFFERENCE ALGORITHM FOR THE ONE-DIMENSIONAL TRANSPORT-DIFFUSION EQUATION
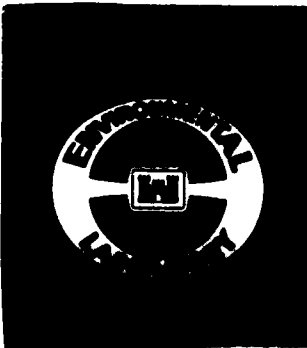
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A stable, accurate, and robust finite-difference algorithm has been successfully developed for engineering solution of the one-dimensional transport-diffusion equation. It is implicit and accurate to a higher order through removal of truncation errors, and uses quadratic upstream weighted differencing of the advection term to eliminate wiggle instabilities. Patterned after the ──> cont

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20. ABSTRACT (Continued).

explicit scheme, the implicit method essentially doubles the useful, stable range of application with comparable accuracy.

Because of these significant improvements for one-dimensional problems, it is strongly recommended that the implicit method be extended to two dimensions.

PREFACE

This report was prepared by Dr. David R. Basco, Department of
Civil Engineering, Texas A&M University Research Foundation, for the
U. S. Army Engineer Waterways Experiment Station (WES) under Contract
No. DACW39-81-M-4377 dated 19 August 1981. The study was sponsored by
the Office, Chief of Engineers, under the Environmental Impact Research
Program (EIRP) Work Unit 31730. The purpose of the report was to investi-
gate the formulation and stability of implicit formulations of QUICKEST.
The report is directed toward personnel with an understanding of finite
differences.

The study was monitored at WES by Mr. Ross Hall, Environmental Re-
search and Simulation Division (ERSD), Environmental Laboratory (EL).
Mr. Donald Robey, Chief, ERSD, and Dr. John Harrison, Chief, EL, pro-
vided supervision. Dr. Roger Saucier was Program Manager, EIRP;
Mr. John Bushman was Technical Monitor.

Commander and Director of WES during report preparation was COL
Tilford C. Creel, CE. Technical Director was Mr. F. R. Brown.

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NOMENCLATURE

a,b,k,h	Variables in two-dimensional Taylor series expansion method
A	Amplification factor in linear stability method, A = modulus; coefficient in QUICK method of Leonard (1979)
A,B,C1,D,E,F,H	Coefficients in implicit, finite-difference methods
C	Courant number
CURV	Curvature
e	A subscript meaning $\underline{e}$xact equation
GRAD	Gradient
H.O.T.	Higher order truncation error terms
i	Space step index
$\overset{o}{\Pi}$	Imaginary number index
JW	One half the base width of the test triangle
κ	Wave number, $2\pi/L$
K	Diffusion (dispersion) coefficient
ℓ	Left side wall value as subscript
L.	Wave length
n	Time step index as superscript; also *number of Taylor series terms*
N	Total number of grid points in one full wave length
NN	Total number of time steps
P_Δ	Péclét number
Q	Phase ratio
r	Right side wall value as subscript
R_e	Exact continuum response function
RMS	Root-mean-square value
t	Time; as subscript means time differentiation
Δt	Time step
u	Velocity
x	Space coordinate; as subscript means space differentiation
Δx	Space step
①,②,③, etc.	Truncation error terms

1-D	One-dimensional
2-D	Two-dimensional
α	Dimensionless wave number
Γ	Dimensionless diffusion coefficient (the diffusion number)
θ	Weighting factor, $0 \le \theta \le 1$ in implicit schemes
ϕ	Dependent variables

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AN IMPLICIT, WIGGLE-FREE, AND ACCURATE UPSTREAM FINITE-DIFFERENCE ALGORITHM FOR THE ONE-DIMENSIONAL TRANSPORT-DIFFUSION EQUATION

PART I: INTRODUCTION

1. Implicit finite-difference algorithms use more than one un-
known variable at the next time level (n+1) in the calculation. They
thereby require the simultaneous solution of many equations at time
(n+1) in order to advance the computation for marching-type, initial
value/boundary value problems.

2. In general, implicit schemes have better stability properties
than explicit schemes. For propagation-dominated problems, this means
running with Courant numbers greater than unity to use more economic
time steps in the computation. In general, the price paid is less accu-
racy and larger Central Processing Unit (CPU) times on the computer. In
addition, implicit schemes require a prescribed order or direction of
the computation in the space of the independent variables. This can be
called the algorithmic structure of the scheme (Abbott 1979). Use of an
inappropriate structure will result in an ill-posed problem and unstable
solution.

3. Eng ers require robust schemes in their computational sys-
tems to pr   greater flexibility in use, yet maintain acceptable
standards or _ccuracy over a wide variety of conditions. Properly de-
signed implicit schemes have met these needs in many aspects of Compu-
tational Hydraulics.

4. For transport-diffusion computations, Leonard (1979) has de-
veloped the explici⁺ QUICKEST modeling procedure. It avoids the "wiggle"
instability problem associated with central differencing of the advec-
tion term. It also eliminates the inaccuracies of numerical diffusion
resulting when only first-order, upstream differencing procedures are em-
ployed. The purpose of this research effort was to develop and study
numerical properties of an implicit algorithm consistent with the Leonard
(1979) scheme for the one-dimensional transport-diffusion equation.

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5. Part II of this report reviews the explicit scheme of Leonard (1979) and proves its equivalence to first-order differences with judicious removal of the truncation error terms. In Part III, two implicit schemes are developed and their characteristics are investigated using linear stability analysis methods and standard numerical tests. Both implicit methods are then compared with the explicit Leonard scheme. Conclusions and recommendations follow in Part IV.

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6. It is highly instructive to briefly review Leonard's (1979) explicit scheme for unsteady transport diffusion, which is labeled QUICKEST (quadratic upstream interpolation for convective kinematics with estimated streaming terms). Consider the differential equation

$$\phi_t + u\phi_x = K\phi_{xx} \qquad\qquad u,K \text{ real constants} \qquad (1)$$

together with appropriate initial and boundary conditions.* A scalar quantity ϕ is convected by constant velocity u and diffused by a constant diffusion coefficient K in one space dimension. A source term could also be added, if necessary.

7. For the finite-difference grid shown in Figure 1, Leonard (1979) proposed using a basic, three-point, upstream-weighted, quadratic interpolation scheme for "wall" values ϕ_r (right) and ϕ_ℓ (left) of a control volume when u is positive to the right. For steady-state conditions, Leonard took
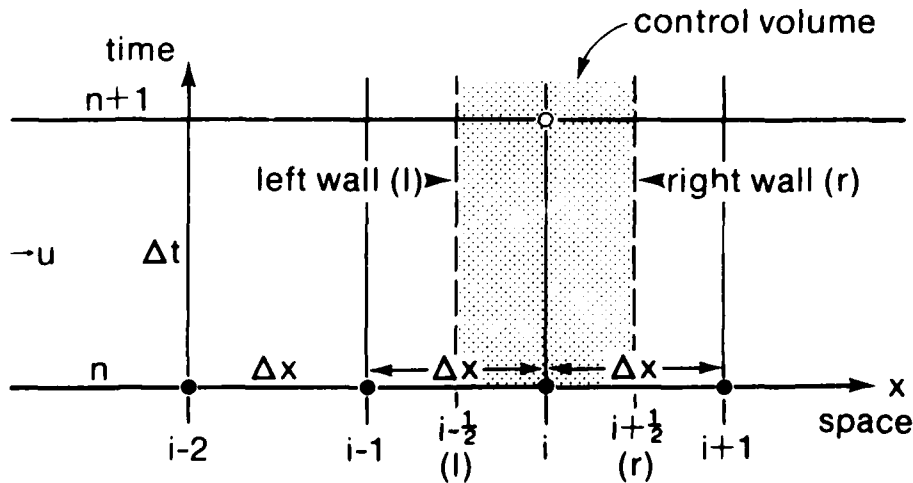
Figure 1. Schematic of QUICKEST algorithm for flow from
left to right

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* See "Nomenclature" on page 5 for definitions of symbols and abbreviations.

$$\phi_r = \phi_{i+1/2} = 1/2(\phi_{i+1} + \phi_i) - A(\phi_{i+1} - 2\phi_i + \phi_{i-1}) \tag{2}$$

$$\phi_\ell = \phi_{i-1/2} = 1/2(\phi_i + \phi_{i-1}) - A(\phi_i - 2\phi_{i-1} + \phi_{i-2}) \tag{3}$$

with A = 1/8 for steady flows (QUICK algorithm).

8. For unsteady-state conditions, Equations 2 and 3 were incorporated in an exact integral formulation where average wall values over time increment Δt were employed. Complete details are beyond the intended scope of this review.

Explicit Operator (QUICKEST)

9. The resultant explicit, finite-difference operator for the QUICKEST algorithm becomes (Leonard 1979, p. 80, Equation 57)

$$
\begin{aligned}
\phi_i^{n+1} = \phi_i^n - C &\left\{ \left[1/2\left(\phi_{i+1}^n + \phi_i^n\right) - \frac{\Delta x}{2} C \cdot GRAD_r - \frac{\Delta x^2}{6}(1 - C^2 - 3\Gamma)CURV_r \right] \right. \\
&\left. - \left[1/2\left(\phi_i^n + \phi_{i-1}^n\right) - \frac{\Delta x}{2} C \cdot GRAD_\ell - \frac{\Delta x^2}{6}(1 - C^2 - 3\Gamma)CURV_\ell \right] \right\} \\
&+ \Gamma \left[\left(\Delta x GRAD_r - \frac{\Delta x^2}{2} C \cdot CURV_r \right) - \left(\Delta x GRAD_\ell - \frac{\Delta x^2}{2} C \cdot CURV_\ell \right) \right]
\end{aligned} \tag{4}
$$

where:

$$C = \frac{u\Delta t}{\Delta x} = \text{the Courant Number}$$

$$\Gamma = \frac{K\Delta t}{\Delta x^2} = \text{the dimensionless diffusion coefficient, or the diffusion number}$$

$$GRAD_r = \frac{\phi_{i+1}^n - \phi_i^n}{\Delta x}$$

$$CURV_r = \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i+1}^n}{\Delta x^2}$$

$$GRAD_\ell = \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}$$

$$CURV_\ell = \frac{\phi_i^n - 2\phi_{i-1}^n + \phi_{1-2}^n}{\Delta x^2}$$

for flow from left to right for both walls (r = right; ℓ = left). Note that for this case, both curvature terms CURV are actually centered upstream by one-half increment and not at r or ℓ as indicated. This is a key aspect of the QUICKEST scheme. In Equation 4, the physical diffusion is calculated using a standard, centered, second difference operator at point i. The overall (global) truncation error is third order in space, and the scheme gives a conservative formulation with no wiggle instabilities present.

Equivalence to a Higher Order Accuracy Method

10. As shall be demonstrated below, QUICKEST is equivalent to a forward-time, centered-space (FTCS) scheme in which the truncation errors resulting from all terms are subtracted out in a prescribed manner.

11. From a Taylor's series expansion about point (i,n) in Figure 1, one obtains the finite-difference analog to Equation 1.

$$\overset{①}{\left[\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t}\right]} + u \overset{③}{\left[\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}\right]} = K \overset{⑤}{\left[\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}\right]}$$

$$\overset{②}{} + \left[\frac{\Delta t}{2!}\phi_{tt} + \frac{\Delta t^2}{3!}\phi_{ttt} + \frac{\Delta t^3}{4!}\phi_{tttt} + H.O.T.\right]_i^n$$

$$\overset{④}{} + u\left[\frac{\Delta x^2}{3!}\phi_{xxx} + \frac{\Delta x^4}{5!}\phi_{xxxxx} + H.O.T.\right]_i^n$$

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$$- K \left[\frac{2\Delta x^2}{4!} \phi_{xxxx} + \frac{2\Delta x^4}{6!} \phi_{xxxxxx} + \text{H.O.T.} \right]_i^n \qquad (5)$$

A forward-time difference (term ①) and a centered-space difference (term ③) are employed along with a centered, second difference (term ⑤) for the diffusion. The bracketed terms ②, ④, and ⑥ are the truncation errors associated with terms ①, ③, and ⑤, respectively.

12. To eliminate the time derivatives in ②, Equation 1 can be further differentiated in time and space to yield

$$\phi_{tt} = u^2 \phi_{xx} - 2uK\phi_{xxx} \qquad (6)$$

$$\phi_{ttt} = -u^3 \phi_{xxx} \qquad (7)$$

and

$$\phi_{tx} = -u\phi_{xx} + K\phi_{xxx} \qquad \text{(a)}$$

$$\qquad (8)$$

$$\phi_{xtt} = u^2 \phi_{xxx} \qquad \text{(b)}$$

when 4th derivatives are neglected. Equation 8 will be used later in this report. Substituting Equations 6 and 7 into 5 and grouping like-ordered differentials gives

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u \left[\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} \right] = K \left[\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i+1}^n}{\Delta x^2} \right]$$

$$+ \frac{u^2 \Delta t}{2!} \left[\phi_{xx} \right]_i^n + \left(\frac{u\Delta x^2}{6} - \frac{u^3 \Delta t^2}{6} - \frac{2uK\Delta t}{2} \right) \left[\phi_{xxx} \right]_i^n$$

$$+ \left[\frac{\Delta t^3}{4} \phi_{tttt} - \frac{2K\Delta x^2}{4!} \phi_{xxxx} + \text{H.O.T.} \right]_i^n \qquad (9)$$

The last bracketed term in Equation 9 is the truncation error

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$O(\Delta t^3, \Delta x^2)$ and contains fourth-order and higher differentials which are neglected. Multiplying through by Δt and clearing all n-level terms to the right-hand side (RHS) gives

$$\phi_i^{n+1} = \phi_i^n - \frac{C}{2}\left(\phi_{i+1}^n - \phi_{i-1}^n\right) + \Gamma\left(\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n\right)$$
$$+ C\left[\frac{C\Delta x^2}{2}\phi_{xx} + \frac{\Delta x^2}{6}\left(\Delta x - C^2\Delta x - 6\Gamma\Delta x\right)\phi_{xxx}\right]_i^n \tag{10}$$

The bracketed term in Equation 10 is the remaining truncation error below ϕ_{xxx} and the method in which it is finite-differenced is central to the equivalency of Equations 4 and 10.

13. Using the terms defined by Leonard (1979) in Equation 4 gives

$$\left(\phi_{xx}\right)_i^n = \frac{GRAD_r - GRAD_\ell}{\Delta x} = \frac{\left[\dfrac{\phi_{i+1}^n - \phi_i^n}{\Delta x}\right] - \left[\dfrac{\phi_i^n - \phi_{i-1}^n}{\Delta x}\right]}{\Delta x}$$

$$= \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}$$

or

$$\Delta x\left(\phi_{xx}\right)_i^n = GRAD_r - GRAD_\ell \tag{11}$$

Thus, for ϕ_{xx}, the centering is precisely at (i,n) as required by Equation 10. Now, if the centering of ϕ_{xxx} is judiciously moved <u>up-stream</u> to $(i - 1/2, n)$, it is assumed that

$$\left(\phi_{xxx}\right)_i^n \doteq \left(\phi_{xxx}\right)_{i-1/2}^n = \frac{CURV_r - CURV_\ell}{\Delta x}$$

$$= \frac{\left[\dfrac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}\right]_i^n - \left[\dfrac{\phi_i^n - 2\phi_{i-1}^n + \phi_{i-2}^n}{\Delta x^2}\right]_{i-1}^n}{\Delta x}$$

$$= \frac{\phi_{i+1}^{n} - 3\phi_{i}^{n} + 3\phi_{i-1}^{n} - \phi_{i-2}^{n}}{\Delta x^3}$$

or

$$\Delta x \left(\phi_{xxx} \right)_{i}^{n} \approx \Delta x \left(\phi_{xxx} \right)_{i-1/2}^{n} = CURV_r - CURV_\ell \qquad (12)$$

The identity

$$\frac{\phi_{i+1}^{n} - \phi_{i-1}^{n}}{2} \equiv 1/2 \left[\phi_{i}^{n} + \phi_{i+1}^{n} \right] - 1/2 \left[\phi_{i}^{n} + \phi_{i-1}^{n} \right] \qquad (13)$$

is also required.

14. Putting Equations 11, 12, and 13 into Equation 10 gives

$$\phi_{i}^{n+1} = \phi_{i}^{n} - C \left[1/2 \left(\phi_{i}^{n} + \phi_{i+1}^{n} \right) - 1/2 \left(\phi_{i}^{n} + \phi_{i-1}^{n} \right) \right] + \Gamma \left[\left(\Delta x GRAD_r \right) \right.$$

$$\left. - \left(\Delta x GRAD_\ell \right) \right] + C \left[\frac{C}{2} \Delta x \left(GRAD_r - GRAD_\ell \right) \right.$$

$$\left. + \frac{\Delta x^2}{6} \left(1 - C^2 - 6\Gamma \right) \left(CURV_r - CURV_\ell \right) \right] \qquad (14)$$

The final trick to recover the form given by Leonard is to split the last term in Equation 14 simply by taking

$$-6\Gamma = -3\Gamma - 3\Gamma$$

and through some further rearrangement. Equation 4 is thus recovered and the derivation is complete.

15. For programming purposes, a much simpler version can be obtained by inserting the difference Equations 11 and 12 for ϕ_{xx} and ϕ_{xxx} , respectively. After grouping all like terms, one obtains

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$$\phi_i^{n+1} = \phi_i^n + \left[-\frac{C}{2} + \Gamma + \frac{C^2}{2} + \frac{C}{6} \left(1 - C^2 - 6\Gamma\right) \right] \phi_{i+1}^n$$

$$- \left[2\Gamma + C^2 + \frac{C}{2} \left(1 - C^2 - 6\Gamma\right) \right] \phi_i^n + \left[\frac{C}{2} + \Gamma + \frac{C^2}{2} \right.$$

$$\left. + \frac{C}{2} \left(1 - C^2 - 6\Gamma\right) \right] \phi_{i-1}^n - \left[\frac{C}{6} \left(1 - C^2 - 6\Gamma\right) \right] \phi_{i-2}^n \qquad (15)$$

16. The algorithm for QUICKEST does reduce to that given by
Leonard (1979) for the steady-state algorithm (QUICK) when term ② for
time derivative truncation error is omitted. Thus QUICKEST *implicitedly*
takes $A = 1/6$ in Equations 2 and 3. Other reduced forms are

Pure Advection ($\Gamma = 0$)

$$\phi_i^{n+1} = \phi_i^n - \frac{C}{6} (C^2 - 3C + 2) \phi_{i+1}^n + \frac{C}{2} (C^2 - 2C - 1)\phi_i^n$$

$$- \frac{C}{2} (C^2 - C - 2) \phi_{i-1}^n + \frac{C}{6} (C^2 - 1)\phi_{i-2}^n \qquad (16)$$

Pure Diffusion ($C = 0$)

$$\phi_i^{n+1} = \phi_i^n + \Gamma \left(\phi_{i+1}^n - 2\phi_i^n + \phi_{i+1}^n \right) \qquad (17)$$

When $\Gamma = 0$ and $C = +1$, Equation 16 reduces to $\phi_i^{n+1} = \phi_{i-1}^n$ or
point-to-point transport for an exact result.

Linear Stability Analysis

17. As a further review and check of these results, a von *Neumann*
linear stability analysis was made of Equation 15. This resulted in the
following expression for the amplification factor A

$$A(\alpha) = 1 + 2(\Gamma + \frac{1}{2} C^2)(\cos \alpha - 1)$$

$$+ \left[\frac{1}{6} C(1 - C^2 - 6\Gamma)(4 \cos \alpha - 3 - \cos 2\alpha) \right]$$

$$- \mathring{\Pi} C \left[\sin \alpha + \frac{1}{6} (1 - C^2 - 6\Gamma)(2 \sin \alpha - \sin 2\alpha) \right] \qquad (18)$$

where:

$\alpha = \kappa\Delta x$ = the dimensionless wave number

κ = the wave number $\frac{2\pi}{L}$

$\alpha = \frac{2\pi}{N}$

N = the number of grid intervals per wave length L

$\overset{o}{\Pi}$ = the imaginary number index

Equation 18 is identical to that derived by Leonard (1979, p. 81, Equation 59), which gives further confidence in these results.

18. An example amplitude portrait for the pure advection case is shown in Figure 2 for three values of the Courant number. The modulus of A versus α plot (Figure 2a) gives more resolution for the higher wave numbers ($\alpha \to \pi$) and consequently has been employed for all subsequent portraits. No phase errors exist for C = 0.5 and 1.0 ($\Gamma = 0$) .

19. The complete stability range in the (Γ,C) plane for the QUICKEST algorithm as mapped by Leonard (1979) is reproduced in Figure 3. Lines of constant Péclét number P_Δ defined as

$$P_\Delta = \frac{C}{\Gamma} \tag{19}$$

are also shown. When $\Gamma = 0$ ($P_\Delta = \infty$) , the QUICKEST scheme is unstable when 1 < C < 2 and also for C > 2 . The scheme is stable for all other Γ, C values within the space shown with the P_Δ lines. Although this explicit scheme is stable for a considerable range above C = 1 , it also is unstable in a "corner" beyond $\Gamma = 0.5$ and below C = 0.5 . It would be anticipated that an implicit version would eliminate this unstable corner.

20. But Figure 3 reveals nothing about the accuracy of the scheme. For the continuum Equation 1, the exact amplitude response function $R_e(\alpha)$ is given by

$$R_e(\alpha) = \exp(-\Gamma\alpha^2) \tag{20}$$

since the modulus for pure advection alone is unity over all α . The exact phase ratio Q_e is also unity for all α since pure diffusion has
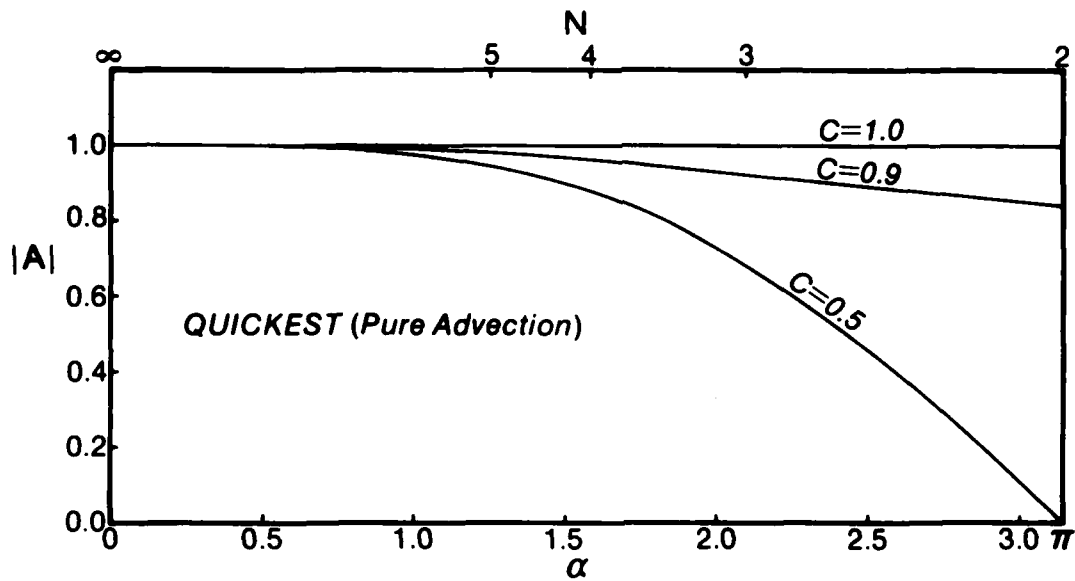
(a) When wave number space is defined by α .
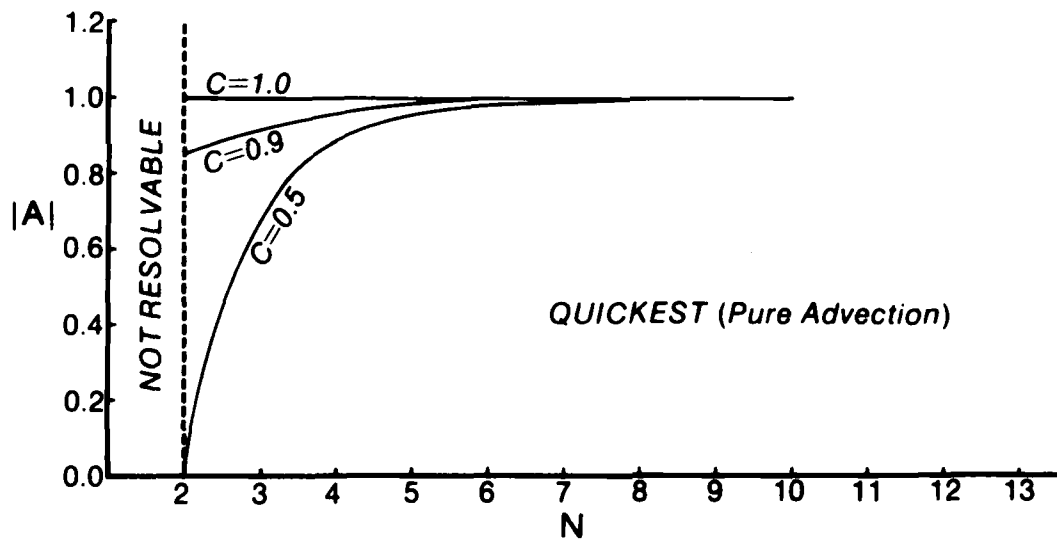
(b) When wave number space is defined by N .

Figure 2. Amplitude portraits of QUICKEST for C = 1.0,
0.9, and 0.5 for pure advection ($\Gamma = 0$)
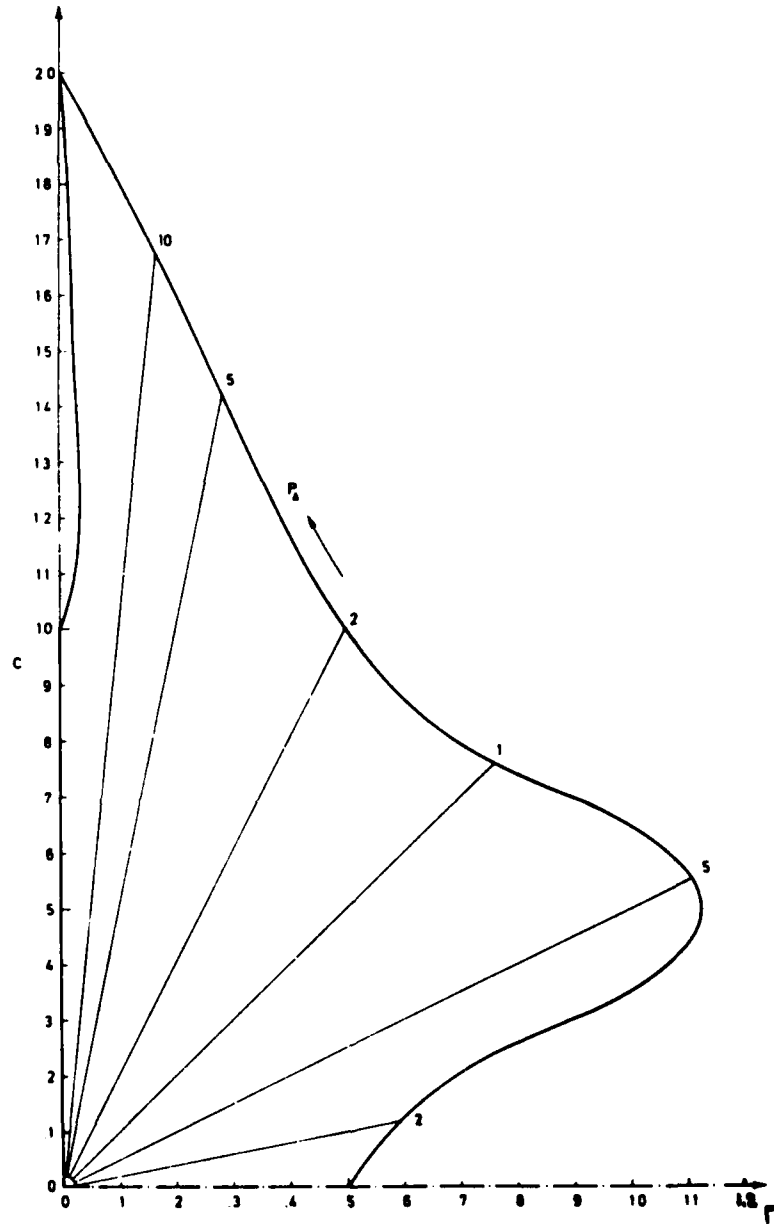
Figure 3. Stability range of QUICKEST method in (Γ,C)
plane as mapped by Leonard (1979). Note that the scheme
is unstable for $1 < C < 2$ and again for $C > 2$ when
$$\Gamma = 0$$

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no phase properties. Examples of the accuracy characteristics of QUICK-EST are presented in Figure 4 when $C = 0.5$, $\Gamma = 1.1$ and in Figure 5 for $C = 0.5$, $\Gamma = 1.2$. The exact response is both cases is also presented. For the stable case (1.1, 0.5), large differences occur for both $|A|$ and Q at higher wave numbers meaning low accuracy for these short wave components. The unstable case (1.2, 0.5) is clearly revealed by the amplitude portrait in Figure 5.
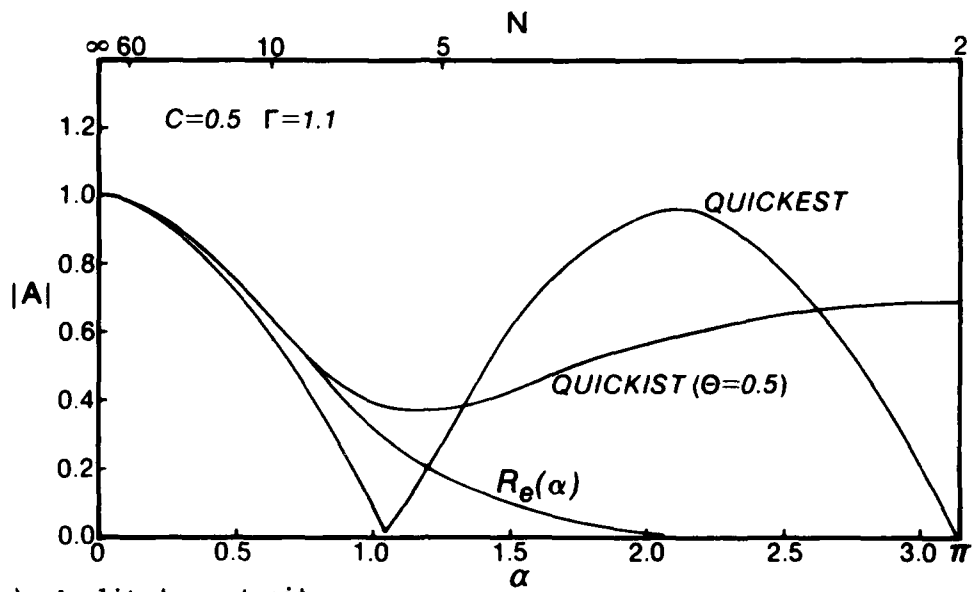
21. It would be very beneficial to characterize the accuracy of QUICKEST by one number over the entire (Γ, C) plane. To do this, the root-mean-square (RMS) value of the differences between continuum (exact) and discrete (approximate) responses was computed using 59 values equally spaced in N . Iso-RMS "difference" lines were then constructed to give the "contour" type plot for amplitude response presented in Figure 6. The weighted-average RMS difference value for the stable area (also traced on Figure 6) is 0.0568. In N-space, this RMS norm was found dependent on the number of differences employed. Further research is needed to refine this approach.

Verification

22. A convenient and informative numerical test for verification of transport-diffusion schemes is the propagation of test triangles with periodic boundary conditions. Since numerical diffusion and convective phase errors are of primary concern, these tests are made with no physical diffusion ($\Gamma = 0$) present. Two examples are shown in Figure 7. Triangles with peak of 1.0 unit centered at $i = 50$ on a 100-unit grid and half-base widths of 20 units (Figure 7a) and 2 units (Figure 7b) are propagated with $C = +0.5$ (left to right). With this Courant number and using periodic boundary conditions, 200 time steps are needed to return the triangle to its initial position shown.

23. The points shown in Figures 7a and 7b are results using the QUICKEST algorithm after 200 time steps. No phase errors are indicated, which confirms the von Neumann analysis. However, numerical amplitude errors for high wave number components cause the peak to be damped,

N

∞ 60   10   5   2

C=0.5 Γ=1.1

1.2

1.0   QUICKEST

0.8

|A| 0.6

0.4   QUICKIST (Θ=0.5)

0.2 $R_e(\alpha)$

0.0
    0   0.5   1.0   1.5   2.0   2.5   3.0 π
                                    α

(a) Amplitude portrait.

1.0

0.0   π

                                      QUICKIST (Θ=0.5)

                            -1.0

Q

                            -2.0   QUICKEST

                            -3.0

                            -4.0
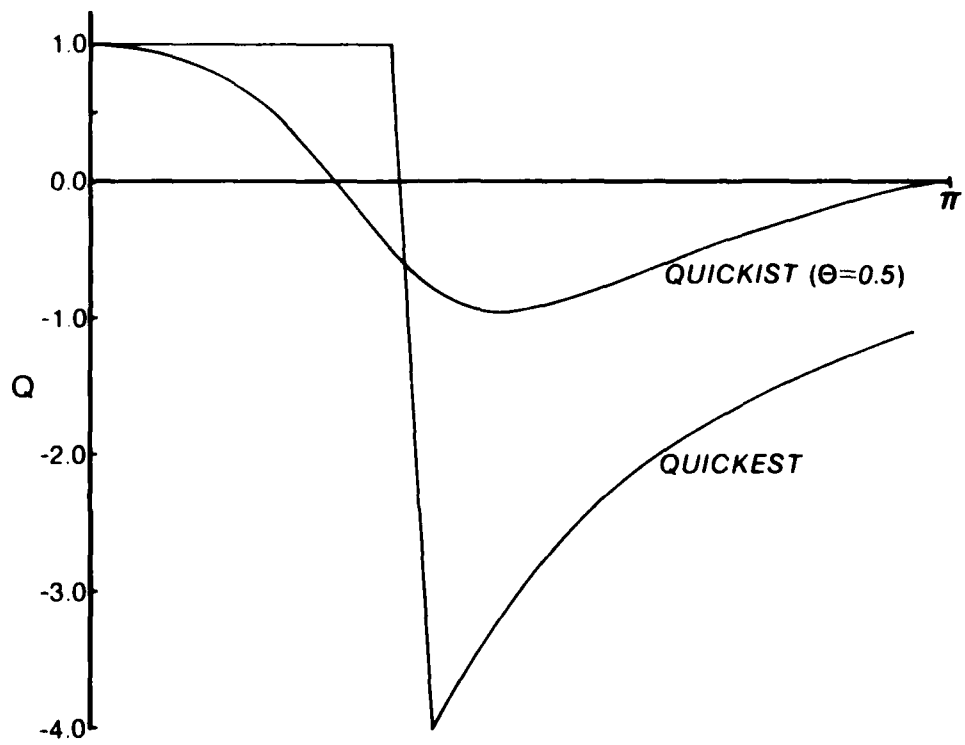
(b) Phase portrait.

Figure 4. Amplitude and phase portraits of QUICKEST and
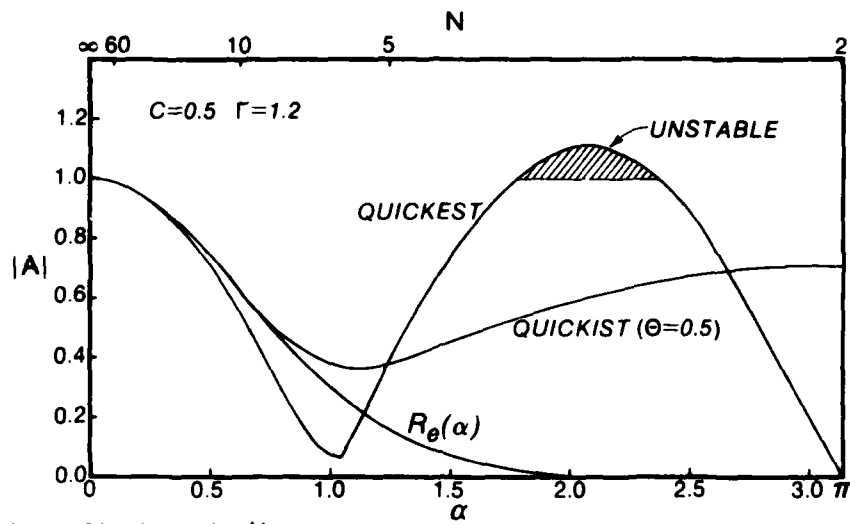QUICKIST (implicit) schemes when C = 0.5 , Γ = 1.1

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(a) Amplitude portrait.
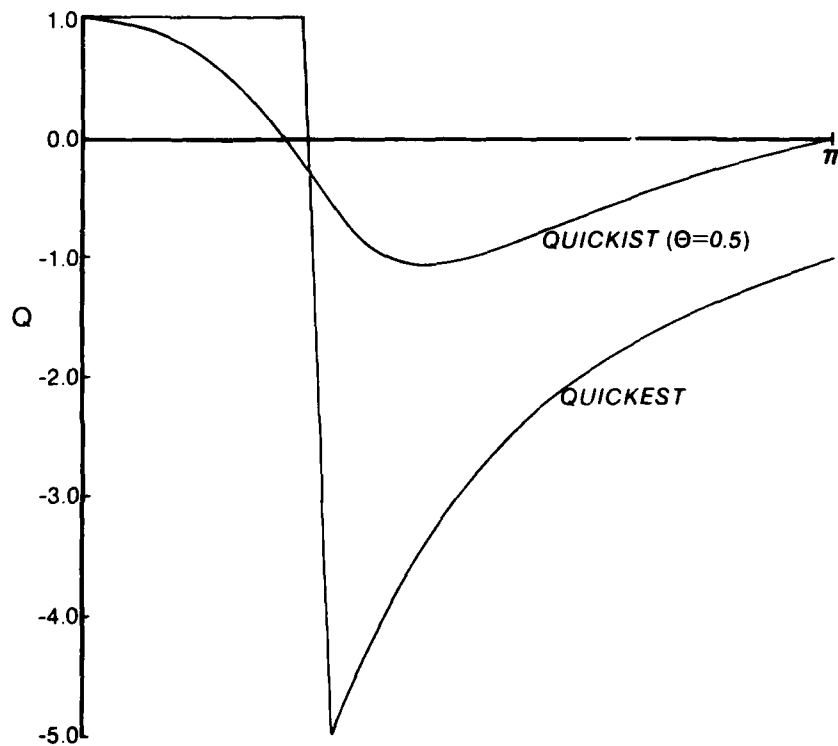

(b) Phase portrait.

Figure 5. Amplitude and phase portraits of QUICKEST and QUICKIST (implicit) schemes when C = 0.5 , Γ = 1.2 . Explicit QUICKEST is unstable

21
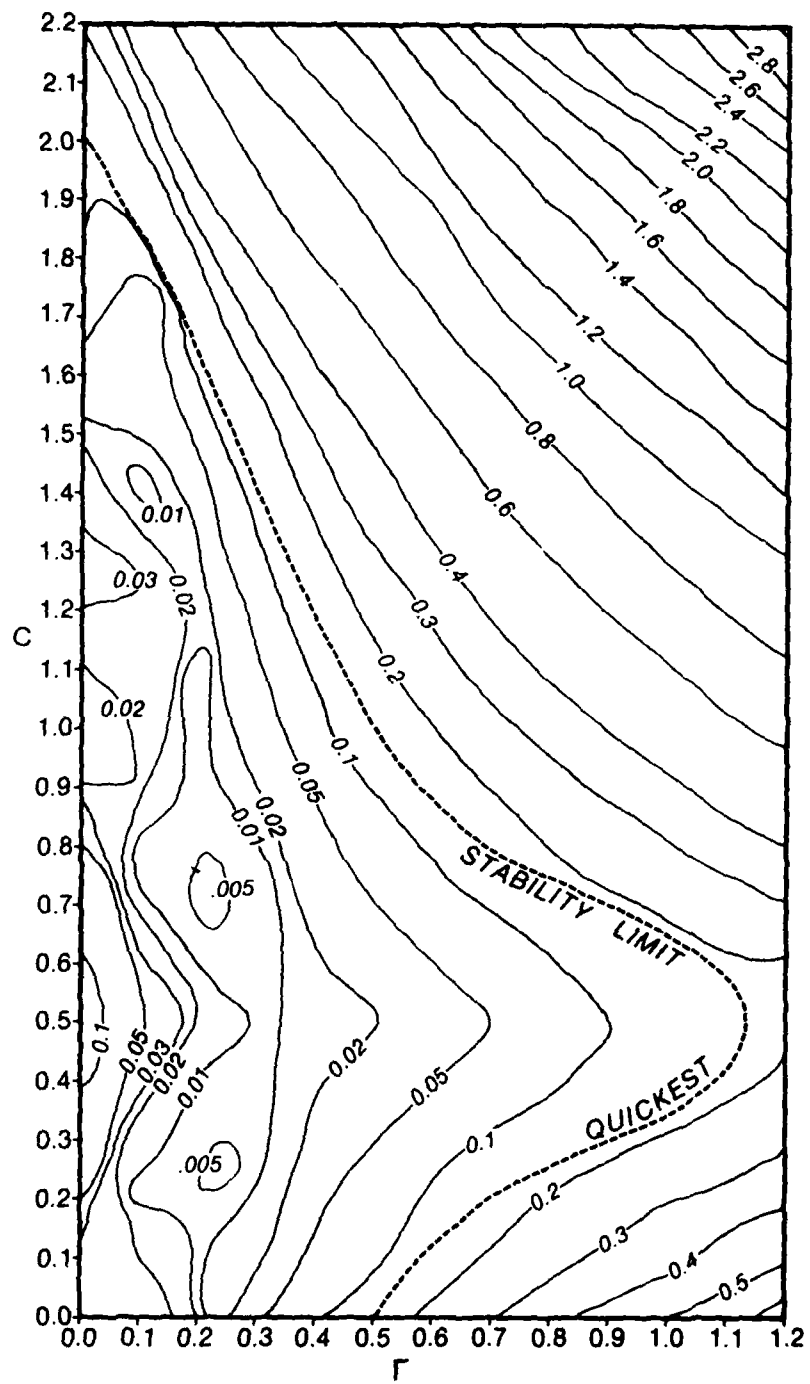
Figure 6. Contour lines of equal RMS difference
values (iso-amplitudes) on the (Γ, C) plane for
QUICKEST. Stability range also shown

22
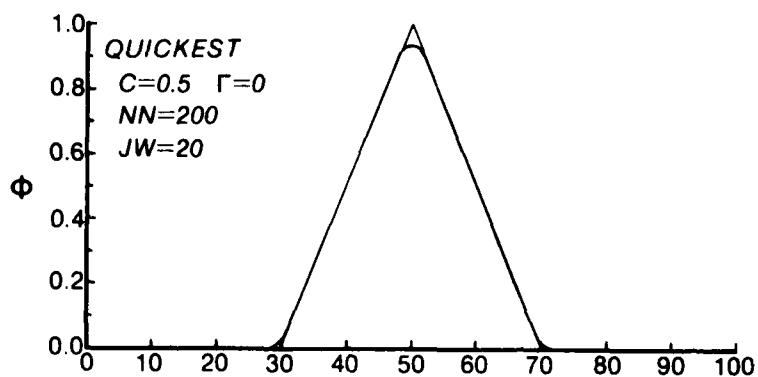
(a) Wide triangle with half-base width of 20 units.
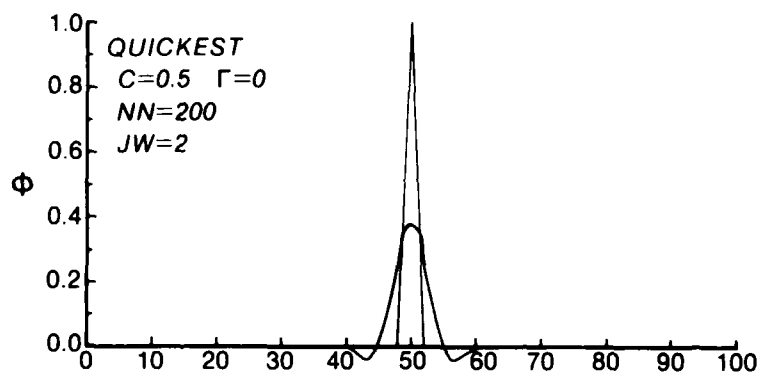
(b) Narrow triangle with half-base width of 2 units.

Figure 7. Propagation test results for pure
advection case using periodic boundary condi-
tions and QUICKEST algorithm with C = 0.5

especially for the "spiked" triangle (JW = 2) example. The damping of
the wider triangle (JW = 20) is relatively minor when compared with that
produced by many first-order finite-difference schemes (see, e.g., Reid
and Basco (1981) for other examples).

Wiggles

24. Wiggles as defined by Leonard (1979) are

"...spatially decaying or growing oscillations of
wavelength $2\Delta x$ (i.e. $\alpha = \pi$, $N = 2$) - typical of
central difference solutions of the...convective-
diffusion problem for $P_\Delta > 2$.

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> ...Interestingly enough, the criterion for the
> absence of wiggles, $P_\Delta \leq 2$, is not a stability
> condition in the von Newmann sense...." (p. 63)

Roache (1977) discusses this as the "zero-overshoot" requirement while
Abbott (1979) mentions "zig-zagging" of free-surface flow schemes. A
full discussion of the sensitivity of the advection term for various
schemes and sensitivity requirements to prevent wiggles is found in
Leonard (1979). Upstream differencing of the advection term always
prevents wiggles.

25. To further examine the wiggle problem for centered convection
schemes, an implicit FTCS scheme was developed with no attempt to remove
the truncation errors. An implicit scheme is necessary for stability
since the explicit FTCS scheme for pure advection is always unstable.
The advection term is centered in space and weighted between n and
n + 1 time levels by a weighting factor $\theta (0 \leq \theta \leq 1)$. The usual
case employed $\theta = 1/2$ to give the $\sigma(\Delta t^2, \Delta x^2)$ for the truncation
error.

26. A linear stability analysis proved the scheme stable for all
(Γ, C) values when $\theta \geq 0.5$. Some phase errors existed, but $|A| \equiv 1$
for all α when $C = 0.5$ and $1.0 (\theta = 1/2)$. Propagation test re-
sults for the wide shape are shown in Figure 8. Clearly, an oscilla-
tion of length $2\Delta x$ is present and can only be explained as a "wiggle"
instability of central differencing since $P_\Delta = \infty$ $(\Gamma = 0)$. In Fig-
ure 8b, the Courant number is 1.0 requiring only 100 time steps to com-
plete the propagation cycle. In each case, the wave moves too slow as
predicted by the phase portrait for higher wave numbers. Additional
tests with $P_\Delta = 2$ eliminated the wiggles. When $P_\Delta = 5$, wiggles
were barely perceptible near the peak as shown in Figure 9, where the
triangles only represent initial conditions since physical diffusion is
now included.

24
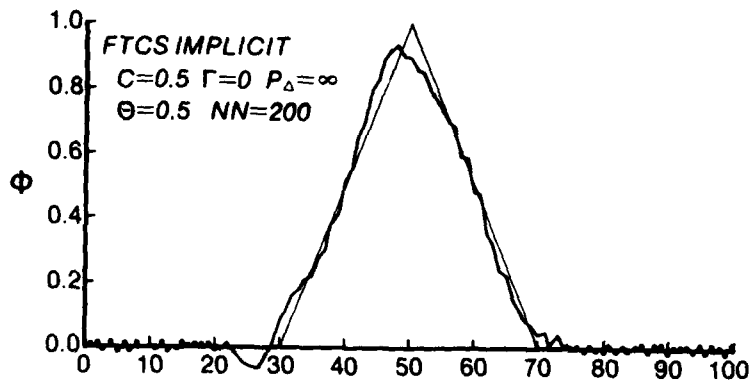
(a) When C=0.5 and after 200 time steps.
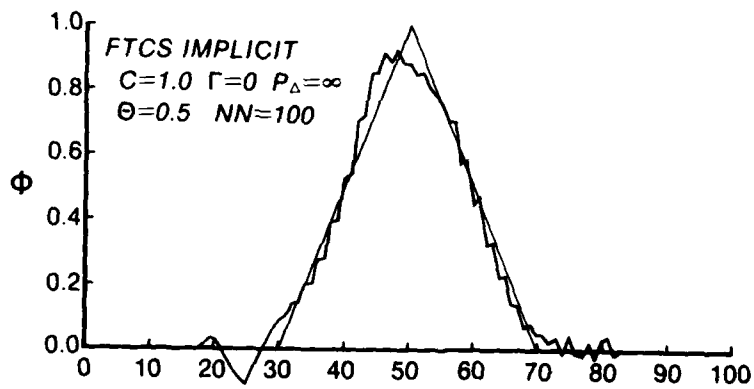
(b) When C=1.0 and after 100 time steps.

Figure 8.   Example of wiggle instability for
implicit, centered advection of test triangle
with periodic boundary conditions

25
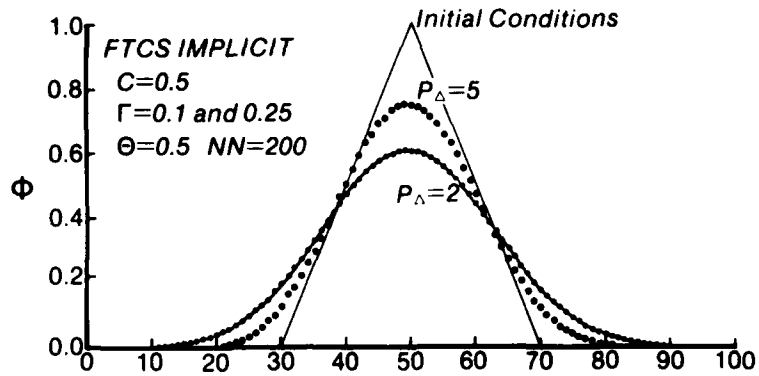
(a) When C=0.5 and after 200 time steps.
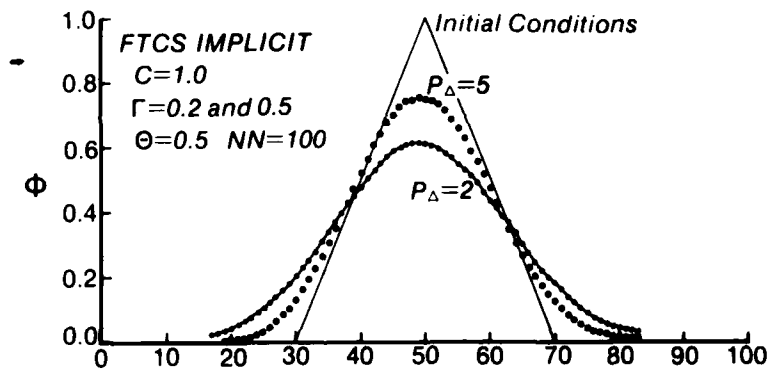
(b) When C=1.0 and after 100 time steps.

Figure 9. Suppression of wiggle instability when $P_\Delta \leq 2$ for implicit, centered advection of test triangle. When $P_\Delta = 5$, a slight oscillation is barely visible

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27. Many alternative ways exist to formulate implicit, higher order accurate difference schemes for Equation 1. Two methods are described below, both of which utilize elements of the explicit, Leonard (1979) algorithm.

Implicit Leonard Algorithm for Transport-Diffusion (QUICKIST)

28. In discussions of computational efficiency and expense of the QUICK (steady-state) method, Leonard (1979, p. 73) states

> Implicit, tridiagonal procedures are similarly economical. In that case, one merely uses (29),* treating the linear-interpolation term implicitly, with the curvature evaluated as as explicit source term.

As derived in the previous chapter, the linear-interpolation term stems from central differencing the advection term. Consequently, this term is made implicit through use of a weighting coefficient θ such that $0 \leq \theta \leq 1$, i.e.,

$$(1 - \theta)(\phi_x)_i^n = (1 - \theta) \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} - (1 - \phi)\left[\phi_{xxx} \frac{\Delta x^2}{3!} + \phi_{xxxxx} \frac{\Delta x^4}{5!} + H.O.T. \right]_i^n \quad (21)$$

$$\theta(\phi_x)_i^{n+1} = \theta \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} - \theta \left[\phi_{xxx} \frac{\Delta x^2}{3!} + \phi_{xxxxx} \frac{\Delta x^4}{5!} + H.O.T. \right]_i^{n+1} \quad (22)$$

A similar weighting makes the diffusion implicit (Crank-Nicholson method) so that, by analogy to Equation 5,

---

* Equations 2 and 3 in this report.

$$\underset{\text{①}}{\left[\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t}\right]} + u(1-\theta)\underset{\text{③}}{\left[\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}\right]} + u\theta\underset{\text{⑦}}{\left[\frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x}\right]}$$

$$= K(1-\theta)\underset{\text{⑤}}{\left[\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}\right]} + K\theta\underset{\text{⑨}}{\left[\frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2}\right]}$$

$$+ \underset{\text{②}}{\left[\frac{\Delta t}{2!}\phi_{tt} + \frac{\Delta t^2}{3!}\phi_{ttt} + \frac{\Delta t^3}{4!}\phi_{tttt} + \text{H.O.T.}\right]_i^n}$$

$$+ u(1-\theta)\underset{\text{④}}{\left[\frac{\Delta x^2}{3!}\phi_{xxx} + \frac{\Delta x^4}{5!}\phi_{xxxxx} + \text{H.O.T.}\right]_i^n}$$

$$+ u\theta\underset{\text{⑧}}{\left[\frac{\Delta x^2}{3!}\phi_{xxx} + \frac{\Delta x^4}{5!}\phi_{xxxxx} + \text{H.O.T.}\right]_i^{n+1}}$$

$$-K(1-\theta)\underset{\text{⑥}}{\left[\frac{2\Delta x^2}{4!}\phi_{xxxx} + \text{H.O.T.}\right]_i^n} - K\theta\underset{\text{⑩}}{\left[\frac{2\Delta x^2}{4!}\phi_{xxxx}\right]_i^{n+1}} \quad (23)$$

When $\theta = 0$, terms ⑦, ⑧, ⑨, and ⑩ disappear and the explicit
scheme given by Equation 5 is recovered. Again, neglecting all fourth
and higher order derivatives, Equation 23 gives, after rearrangement,

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$$\overset{\textcircled{8}}{}$$

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\theta \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} - u\theta \frac{\Delta x^2}{3!}\left[\phi_{xxx}\right]_i^{n+1} - K\theta \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2}$$

$$= -u(1 - \theta) \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} + K(1 - \theta) \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}$$

$$\overset{\textcircled{4}}{}$$

$$+ u(1 - \theta) \frac{\Delta x^2}{3!} \left[\phi_{xxx}\right]_i^n$$

$$\overset{\textcircled{2a}}{} \qquad\qquad \overset{\textcircled{2b}}{}$$

$$+ \left[\frac{\Delta t}{2}\left(u^2\phi_{xx} - 2uK\phi_{xxx}\right)\right]_i^n + \left[\frac{\Delta t^2}{3!}\left(-u^3\phi_{xxx}\right)\right]_i^n \qquad (24)$$

29. The numbered brackets identify truncation error terms. Truncation error time derivatives are again converted to space derivatives using Equations 6 and 7 to give terms $\textcircled{2a}$ and $\textcircled{2b}$, respectively. All truncation error derivatives are at time level n except term $\textcircled{8}$. A third spatial derivative requires four grid points, which is incompatible with a tridiagonal algorithm. Based on the derivation in the previous chapter and the quote above (Leonard 1979, p. 73), for evaluation of the curvature as an "explicit source term," term $\textcircled{8}$ is taken at time level n . This is a key assumption in this first method. Also, the time derivative is still centered at grid point (i,n) so that this implicit method reduces to the explicit method of Leonard (1979) called QUICKEST when $\theta = 0$. Here the underlined E also could stand for the explicit algorithm. By analogy, for later reference, this implicit algorithm is labeled QUICKIST.

30. Removing term $\textcircled{8}$ in Equation 24 to time level n , multiplying through by Δt , and rearranging by grouping all like terms gives

$$\left(\frac{C\theta}{2} - \Gamma\theta\right)\phi_{i+1}^{n+1} + (1 + 2\Gamma\theta)\phi_i^{n+1} - \left(\frac{C\theta}{2} + \Gamma\theta\right)\phi_{i-1}^{n+1}$$

$$= \left[-\frac{C(1-\theta)}{2} + \Gamma(1-\theta)\right]\phi_{i+1}^n + \left[1 - 2\Gamma(1-\theta)\right]\phi_i^n$$

$$+ \left[\frac{C(1-\theta)}{2} + \Gamma(1-\theta)\right]\phi_{i-1}^n + \left[\frac{C^2\Delta x^2}{2}\right][\phi_{xx}]_i^n$$

$$+ \left[\underbrace{\frac{C\Delta x^3}{6}(1-\theta) + \frac{C\Delta x^3}{6}\theta}_{\textcircled{8}} - C\Delta x^3\Gamma - \frac{C^3\Delta x^3}{6}\right][\phi_{xxx}]_i^n \qquad (25)$$

Note that taking term $\textcircled{8}$ to level n effectively removes the influence of θ on the truncation errors associated with the convection term.

31. Finally, if again the assumption is made that, inherent in Equation 12 for upstream differencing of left to right flow, $(\phi_{xxx})_i^n \approx (\phi_{xxx})_{i-1/2}^n$, then using Equation 11 plus additional rearrangement gives

$$A\phi_{i+1}^{n+1} + B\phi_i^{n+1} + C1\phi_{i-1}^{n+1} = D\phi_{i+1}^n + E\phi_i^n + F\phi_{i-1}^n + H\phi_{i-2}^n \qquad (26)$$

Where

$$A = \left(\frac{C\theta}{2} - \Gamma\theta\right) \qquad (a)$$

$$B = 1 + 2\Gamma\theta \qquad (b)$$

$$C1 = -\left(\frac{C\theta}{2} + \Gamma\theta\right) \qquad (c)$$

$$D = \left[-\frac{C}{2}(1-\theta) + \Gamma(1-\theta) + \frac{C^2}{2} + \frac{C}{6}(1 - C^2 - 6\Gamma)\right] \qquad (d)$$

$$E = \left[1 - 2\Gamma(1-\theta) - C^2 - \frac{C}{2}(1 - C^2 - 6\Gamma)\right] \qquad (e)$$

$$F = \left[\frac{C}{2}(1-\theta) + \Gamma(1-\theta) + \frac{C^2}{2} + \frac{C}{2}(1 - C^2 - 6\Gamma)\right] \qquad (f)$$

$$H = -\frac{C}{6}(1 - C^2 - 6\Gamma) \qquad (g)$$

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When $\theta = 0$, Equation 26 reduces to Equation 15, as expected. This form is convenient for the linear stability analysis and propagation tests using double-sweep, tridiagonal matrix solution procedures.

Linear stability analysis of QUICKIST

32. Use of the von Neumann method resulted in the following expression for the amplification factor

$$A(\alpha) = \frac{D \exp(\overset{o}{\Pi}\alpha) + E + F \exp(-\overset{o}{\Pi}\alpha) + H \exp(-\overset{o}{\Pi}2\alpha)}{A \exp(\overset{o}{\Pi}\alpha) + B + C1 \exp(-\overset{o}{\Pi}\alpha)} \tag{27}$$

A simple computer program written in complex arithmetic was employed to find $|A|$ and Q over 30 values of α from Equation 27 without further simplification.

33. Some results when $\theta = 0.5$ are shown in Figure 10 for $C = 0.5$ and Figure 11 when $C = 1.0$. In both instances, the explicit
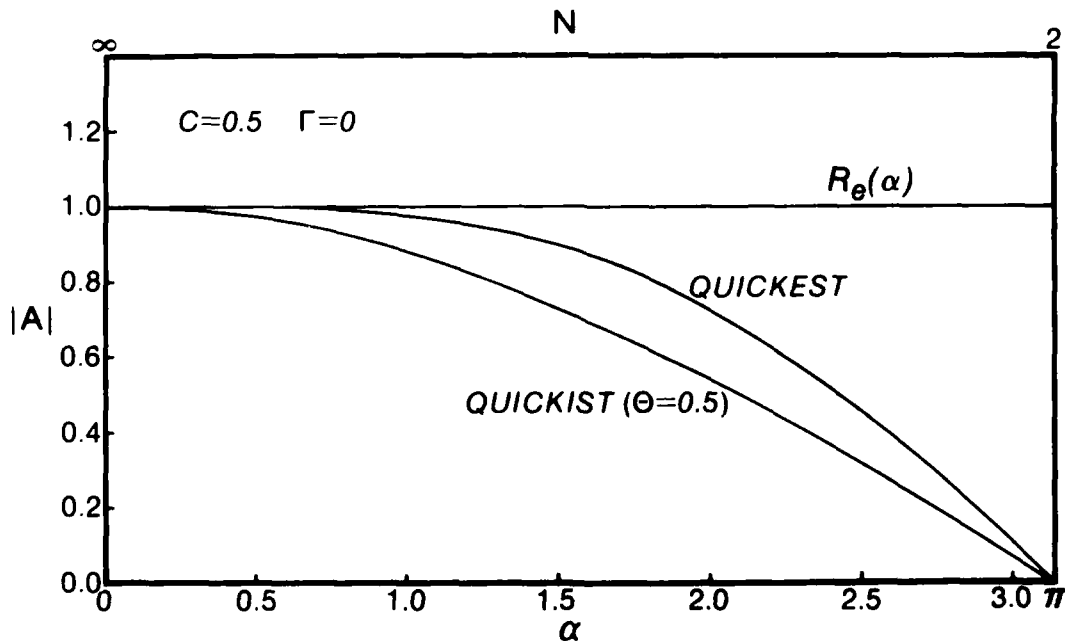

Figure 10. Amplitude portrait for QUICKEST versus QUICKIST schemes when $C = 0.5$, $\Gamma = 0$. Both have no phase errors for all of α
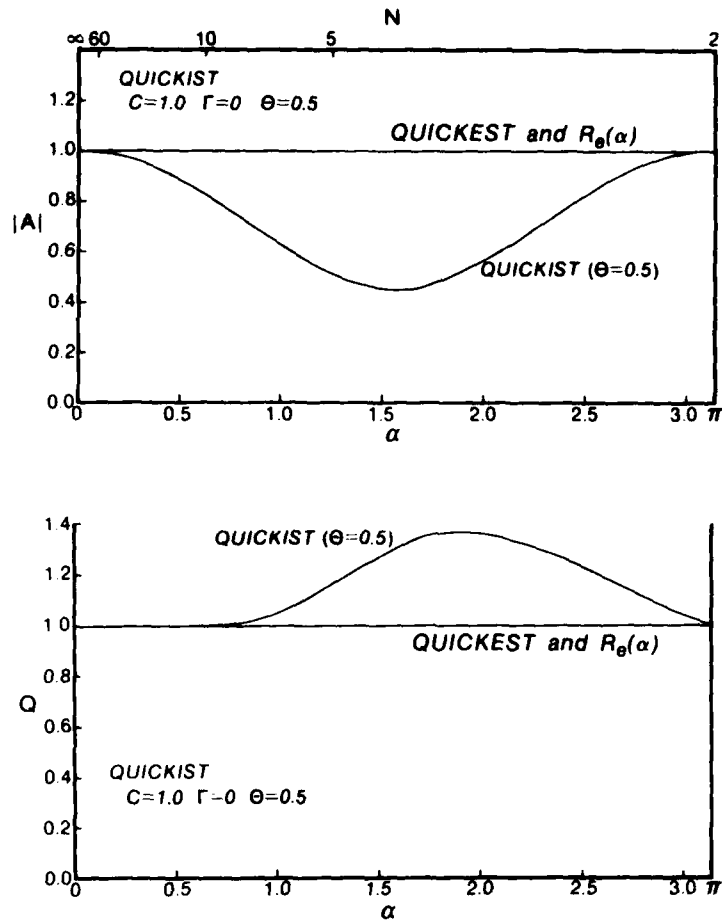
31

Figure 11. Amplitude and phase portraits for QUICKEST and
QUICKIST schemes when C = 1.0 , Γ = 0

scheme is more accurate for pure advection. The extent of numerical
damping when C = 1.0 for the QUICKIST algorithm can be considered ex-
cessive. However, as shown in Figure 4 for C = 0.5 , Γ = 1.1 ,
QUICKIST (θ = 0.5) appears more accurate for all α . Figure 5 also
reveals that when C is again 0.5 but Γ now 1.2, QUICKIST is stable
whereas the explicit scheme is unstable. The implicit algorithm has
far superior phase response for these latter examples. Finally, Fig-
ure 12 reveals that the explicit scheme is more accurate over all α
for the pure diffusion case when Γ = 1/6 .

    34. The (Γ,C) plane was mapped for the implicit scheme to
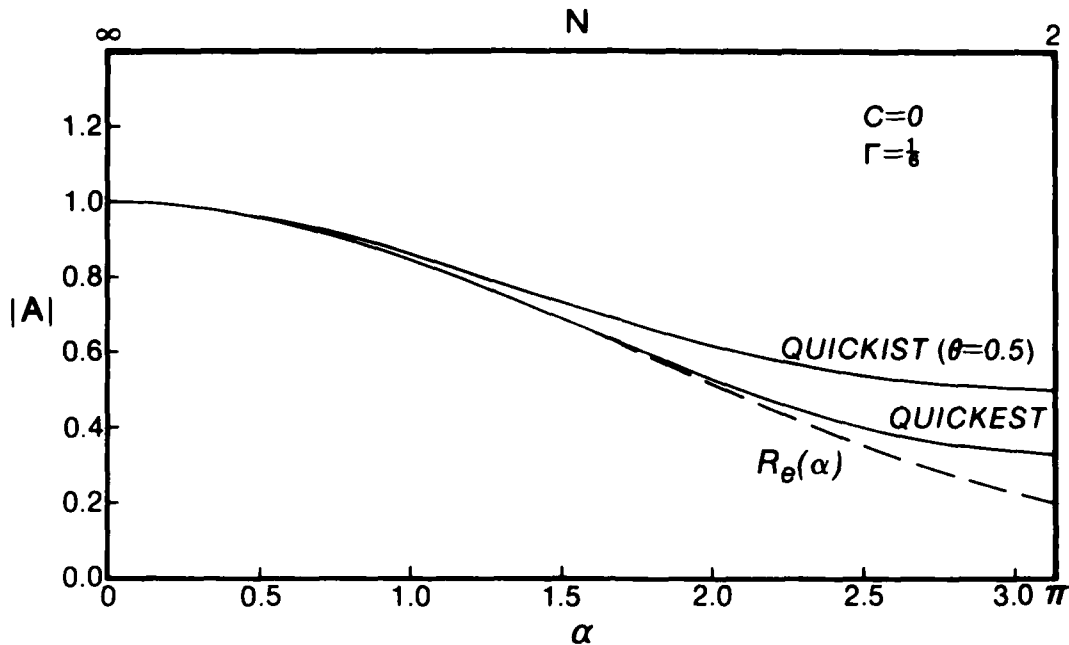
32

Figure 12. Amplitude response for pure diffusion (C = 0) when
Γ = 1/6   for both QUICKEST and QUICKIST schemes

determine its stability range* for comparison with Leonard's results
in Figure 3.   The results were somewhat disappointing.   It was antici-
pated that the implicit QUICKIST algorithm would have a much larger
stable region than shown in Figure 13.   However, the unstable corner
below   C = 0.5   and beyond   Γ = 0.5   was eliminated.   The stable range
of QUICKEST method is also shown in Figure 13 for comparison.

35.   The amplitude accuracy of QUICKIST was characterized in the
stable range out to   Γ = 1.3   using the RMS difference norm, as before.
Figure 14 presents the "contour" map of RMS difference values and gives
a weighted-average value in the stable area (arbitrarily,   Γ ≤ 1.3) of
0.0946.   As expected, QUICKIST with   θ = 0.5   is less accurate than the
explicit Leonard algorithm.

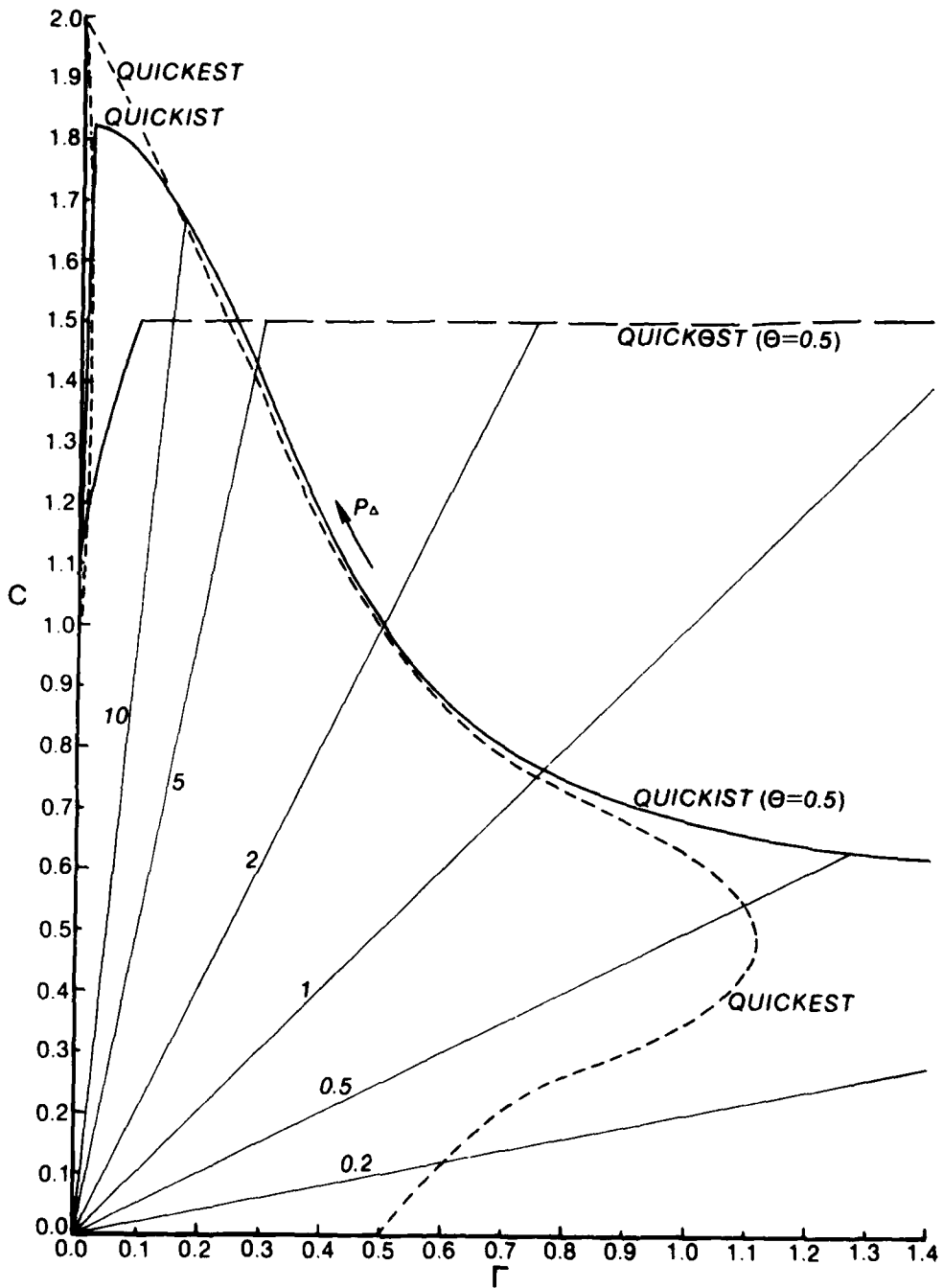* | A | > 1.001 for any $0 \leq \alpha \leq \pi$ was the criteria employed.

Figure 13. Stable range of QUICKIST method in (Γ, C) plane
as determined in this study. Also shown is stable range
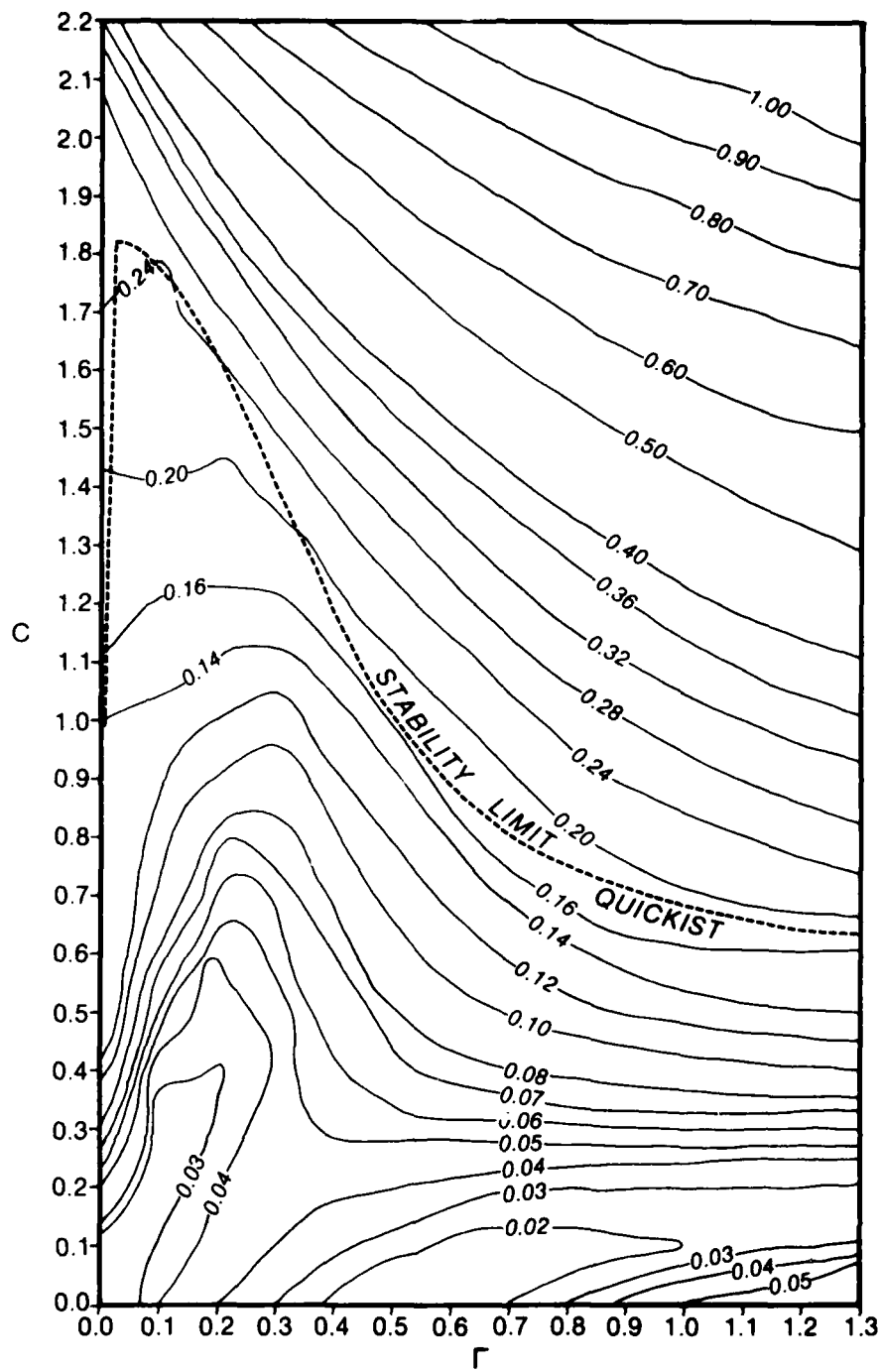of QUICKEST scheme and the QUICKθST algorithm described
later in this report

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Figure 14. Iso-amplitude lines of equal RMS difference values in
(Γ,C) plane for QUICKIST. Stability range also shown

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Propagation tests of QUICKIST

36. The QUICKIST inaccuracies are confirmed by results of the
triangle propagation tests. Excessive numerical damping results to the
extent demonstrated in Figure 15 for C = 0.5 (Fig. 15a) and C = 1.0
(Fig. 15b). When compared with Figure 7 and the fact that C = 1.0
gives an exact result for the explicit scheme, it must be concluded that
the implicit QUICKIST algorithm is too inaccurate to warrant further
study.
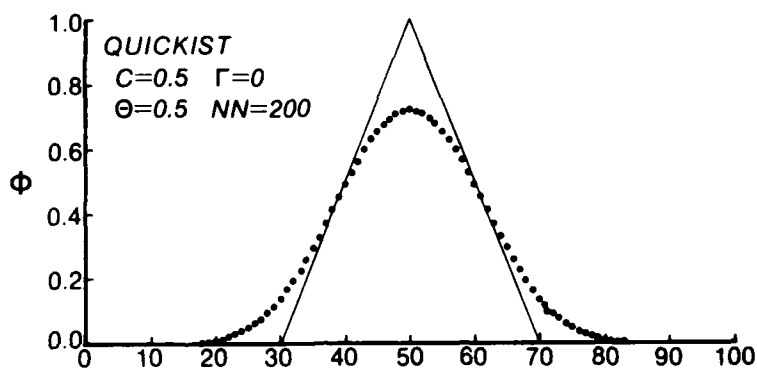
(a) When C=0.5 and after 200 time steps.
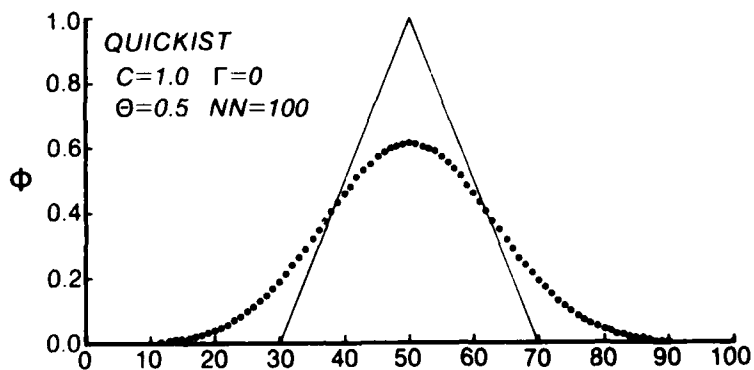
(b) When C=1.0 and after 100 time steps.

Figure 15. Propagation tests for pure advection using
periodic boundary conditions and QUICKIST algorithm.
Large numerical diffusion present

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37. The inaccuracy of the QUICKIST algorithm can be traced to the off-centering of the ϕ_t derivative at (i,n). The sole advantage of this method is that when $\theta = 0$, the explicit QUICKEST algorithm is regained.

38. A fully centered, implicit method would utilize grid point (i,n + 1/2) in the Taylor series expansion so that even the ϕ_t derivative is effectively weighted by θ . When $\theta = 0$, the explicit QUICK-EST scheme would no longer be recovered. However, far greater numerical accuracy is anticipated since all terms and truncation errors are centered at the same time level by θ . Consequently, this fully centered implicit Leonard scheme is given the acronym QUICKθST.

Derivation

39. Consider the schematic grid sketched in Figure 16. A two-dimensional Taylor expansion of the form

$$f(a + h, b + k) = f(a,b) + \left(h \frac{\partial}{\partial x} + k \frac{\partial}{\partial t} \right) f(x,t) \Big|_{\substack{x=a \\ t=b}}$$

$$+ \frac{1}{n!} \left(h \frac{\partial}{\partial x} + k \frac{\partial}{\partial t} \right)^n f(x,t) \Big|_{\substack{x=a \\ t=b}} + \ldots \qquad (28)$$

is utilized where

$$
\begin{aligned}
a &= i \\
b &= n + 1/2 \\
h &= \Delta x \\
k &= \Delta t/2
\end{aligned}
\qquad (29)
$$

for the nomenclature in Figure 16. The initial expansion[*] about (i,n + 1/2) yields by analogy with Equation 23

---

[*] A coefficient was discovered to be missing in this expansion at a later date. The complete results for the correct expansion are given in Appendix A. Surprisingly, the correct expansion (QUICKθST 2 exhibited little if any improvement over the original explicit scheme QUICKEST. Therefore, it was dropped in favor of the "chance" algorithm QUICKθST discussed in detail herein. It was not possible to determine the cause for this unexpected result within the allotted scope of the study.
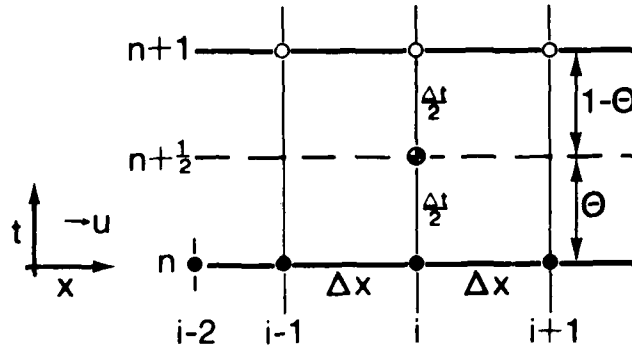
Figure 16. Schematic of operator for QUICKθST
scheme determination

$\textcircled{1}$ $\quad\quad\quad\quad\quad$ $\textcircled{3}$ $\quad\quad\quad\quad\quad$ $\textcircled{7}$

$$\left[\frac{\phi_i^{n+1} - \phi_i^{n}}{\Delta t}\right] + u(1 - \theta)\left[\frac{\phi_{i+1}^{n} - \phi_{i-1}^{n}}{2\Delta x}\right] + u\theta\left[\frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x}\right]$$

$\textcircled{5}$ $\quad\quad\quad\quad\quad$ $\textcircled{9}$

$$= K(1 - \theta)\left[\frac{\phi_{i+1}^{n} - 2\phi_i^{n} + \phi_{i-1}^{n}}{\Delta x^2}\right] + K\theta\left[\frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2}\right]$$

$\textcircled{2}$

$$+ \quad \left[- \frac{1}{24}\Delta t^2 \phi_{ttt} + \text{H.O.T.}\right]_i^{n+1/2}$$

$\textcircled{4}$

$$+ u(1 - \theta)\left[- \frac{1}{2!}\frac{\Delta t}{2}\phi_{xt} + \frac{1}{3!}\Delta x^2 \phi_{xxx} + \frac{\Delta t^2}{24}\phi_{xtt} + \text{H.O.T.}\right]_i^{n+1/2}$$

$\textcircled{8}$

$$+ u\theta\left[\frac{1}{2!}\frac{\Delta t}{2}\phi_{xt} + \frac{1}{3!}\Delta x^2 \phi_{xxx} + \frac{\Delta t^2}{24}\phi_{xtt} + \text{H.O.T.}\right]_i^{n+1/2}$$

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$$\overset{\textstyle\bigcirc\kern-0.9em 6}{} $$

$$- K(1 - \theta) \left[\frac{1}{3!} \, \Delta t \phi_{xxt} + H.O.T. \right]_i^{n+1/2}$$

$$\overset{\textstyle\bigcirc\kern-1.0em 10}{} $$

$$- K\theta \left[\frac{1}{3!} \, \Delta t \phi_{xxt} + H.O.T. \right]_i^{n+1/2} \tag{30}$$

The truncation error terms ②, ④, ⑥, ⑧, and ⑩ are now centered at (i, n + 1/2) giving different coefficients and incorporating mixed time/space derivatives. Neglecting all fourth and higher order derivatives; using Equations 6, 7, and 8 to convert all time and mixed-time derivatives to pure space derivatives; and combining all like derivatives for truncation errors yields

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u(1 - \theta) \, \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} + u\theta \, \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x}$$

$$= K(1 - \theta) \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} + K\theta \, \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2}$$

$$\overset{\textstyle④ + ⑧}{} $$

$$+ \left[\frac{u^2 \Delta t}{4} (1 - 2\theta) \right] \left(\phi_{xx} \right)_i^{n+1/2}$$

$$\overset{\textstyle② + ④ + ⑥ + ⑧ + ⑩}{} $$

$$+ \left[\frac{u\Delta x^2}{6} - \frac{5Ku(1 - 2\theta)\Delta t}{12} \right] \left(\phi_{xxx} \right)_i^{n+1/2} \tag{31}$$

In Equation 31, truncation error from terms ④ and ⑧ contribute to ϕ_{xx} while all truncation error terms contribute to the ϕ_{xxx} coefficient.

40. It is now assumed that:

    <u>a</u>. The truncation errors in Equation 31 are evaluated at time level n .

    <u>b</u>. The ϕ_{xxx} term is centered upstream (grid point (i - 1/2) for left to right flow).

Assumption <u>a</u> is required for ϕ_{xxx} to retain the tridiagonal structure of the algorithm as in QUICKIST. Also, it is felt that for consistency, ϕ_{xx} should also be taken at level n . Assumption <u>b</u> follows from Part II to produce the quadratic, higher order, accurate, upstream difference operator for advection. Using these two assumptions and making the usual rearrangements gives

$$A\phi_{i+1}^{n+1} + B\phi_{i}^{n+1} + C1\phi_{i-1}^{n+1} = D\phi_{i+1}^{n} + E\phi_{i}^{n} + F\phi_{i-1}^{n} + H\phi_{i-2}^{n} \qquad (32)$$

where

$$A = \frac{C\theta}{2} - \Gamma\theta \qquad (a)$$

$$B = 1 + 2\Gamma\theta \qquad (b)$$

$$C1 = -\left(\frac{C\theta}{2} + \Gamma\theta\right) \qquad (c)$$

$$D = \left[-\frac{C}{2}(1 - \theta) + \Gamma(1 - \theta) + \frac{C^2}{4}(1 - 2\theta)\right. \\ \left. + \frac{C}{6} - \frac{5}{12}C\Gamma(1 - 2\theta)\right] \qquad (d)$$

$$E = \left[1 - 2\Gamma(1 - \theta) - \frac{C^2}{2}(1 - 2\theta) - \frac{C}{2} + \frac{15}{12}C\Gamma(1 - 2\theta)\right] \qquad (e)$$

$$F = \left[\frac{C}{2}(1 - \theta) + \Gamma(1 - \theta) + \frac{C^2}{4}(1 - 2\theta)\right. \\ \left. + \frac{C}{2} - \frac{15}{12}C\Gamma(1 - 2\theta)\right] \qquad (f)$$

$$H = -\left[\frac{C}{6} - \frac{5}{12}C\Gamma(1 - 2\theta)\right] \qquad (g)$$

The coefficients D , E , F , and H in Equation 32 are different from the first implicit scheme given by Equation 26. As an example, consider the coefficients when C = 1.0 , $\Gamma = 0$, $\theta = 0.5$

QUICKθST

$$\frac{1}{4}\phi_{i+1}^{n+1} + \phi_{i}^{n+1} - \frac{1}{4}\phi_{i-1}^{n+1} = -\frac{1}{12}\phi_{i+1}^{n} + \frac{6}{12}\phi_{i}^{n} + \frac{9}{12}\phi_{i-1}^{n} - \frac{2}{12}\phi_{i-2}^{n} \qquad (a)$$

QUICKIST

$$\frac{1}{4} \phi_{i+1}^{n+1} + \phi_i^{n+1} - \frac{1}{4} \phi_{i-1}^{n+1} = \frac{1}{4} \phi_{i+1}^{n} + \frac{3}{4} \phi_{i-1}^{n} \qquad\qquad \text{(b) (33)}$$

QUICKEST ($\theta = 0$)

$$\phi_i^{n+1} = \phi_{i-1}^{n} \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(c)}$$

It appears that QUICKθST retains more of the intended upstream interpolation flavor of the Leonard QUICK method.

Linear stability analysis of QUICKθST

41. Equation 27 is again employed but with coefficients calculated from Equation 32. Some results ($\theta = 0.5$) are shown in Figure 17. This implicit scheme is exact in amplitude response for all α when $C = 1.0$ or 0.5 for pure advection. Some phase errors exist for higher wave numbers as demonstrated in Figure 17(b). Figure 17 when compared with Figures 10 and 11 reveals that QUICKθST is vastly superior to QUICKIST and similar to the explicit scheme for these Courant numbers. Both implicit schemes reduce to the Crank-Nicholson scheme for pure diffusion ($C = 0$, $\theta = 0.5$).

42. Mapping the stable area of QUICKθST in the (Γ, C) plane revealed a much larger and uniformly stable region as shown previously in Figure 13. QUICKθST is stable for all Γ below $C = 1.5$ except in the small area above $C = 1.0$ near the ordinate.

43. The amplitude accuracy of QUICKθST is summarized in Figure 18 out to $\Gamma = 1.3$ again using the RMS difference as norm. The weighted-average value in the enlarged stable area ($\Gamma \leq 1.3$) is
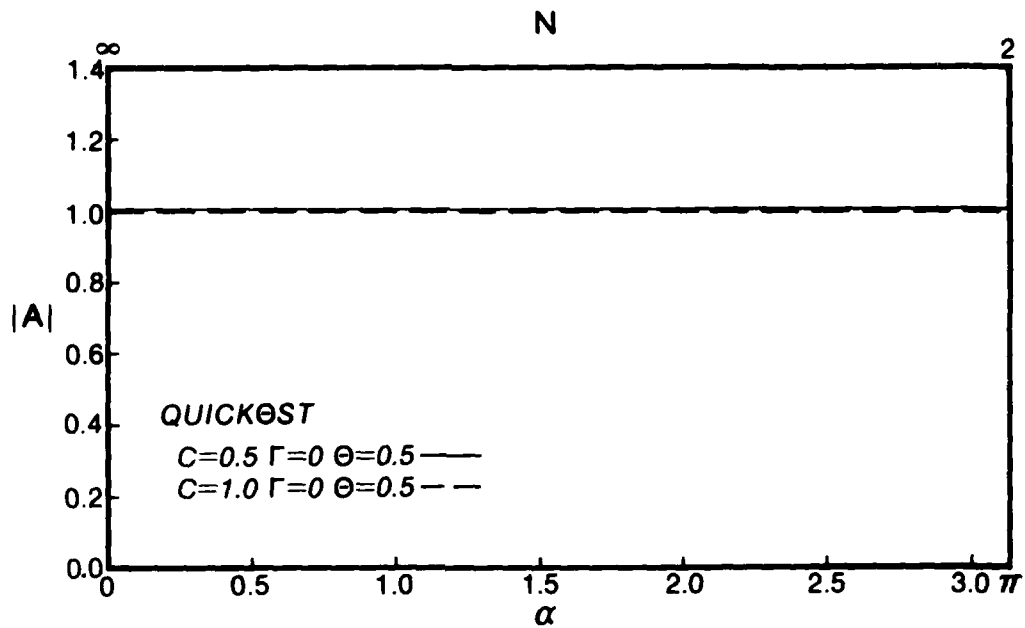
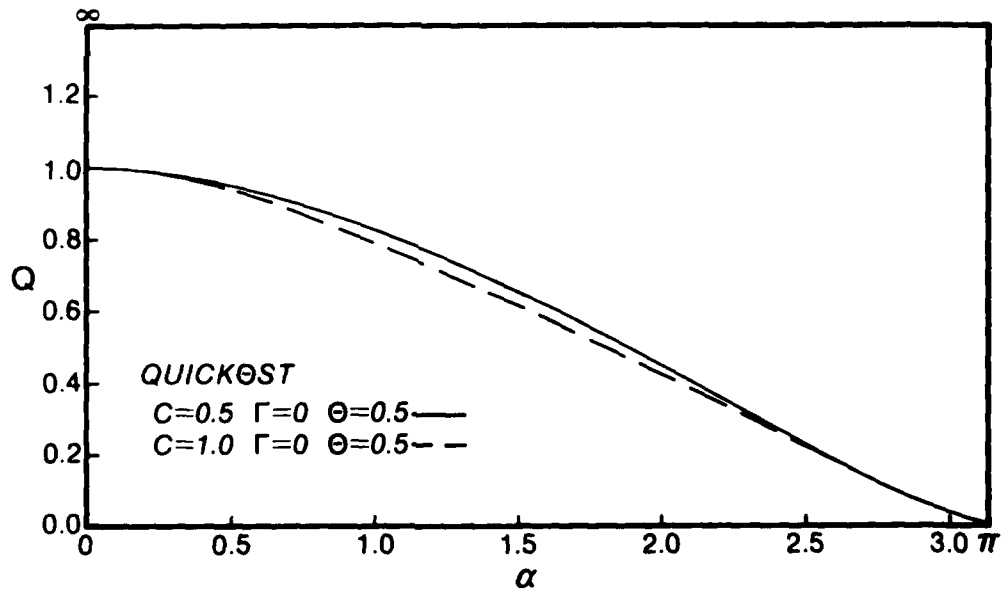QUICKθST   0.0890

and, for comparison,

QUICKIST   0.0946

QUICKEST   0.0568

As expected, the QUICKθST algorithm is more accurate in amplitude response over all wave numbers than QUICKIST. It is generally more inaccurate than the explicit scheme, but is far more useful due to

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(a) Scheme is exact in amplitude response.

(b) Some phase errors present.

Figure 17. Amplitude and phase portraits for QUICKθST scheme and
pure advection (Γ = 0) case when C = 0.5 and 1.0

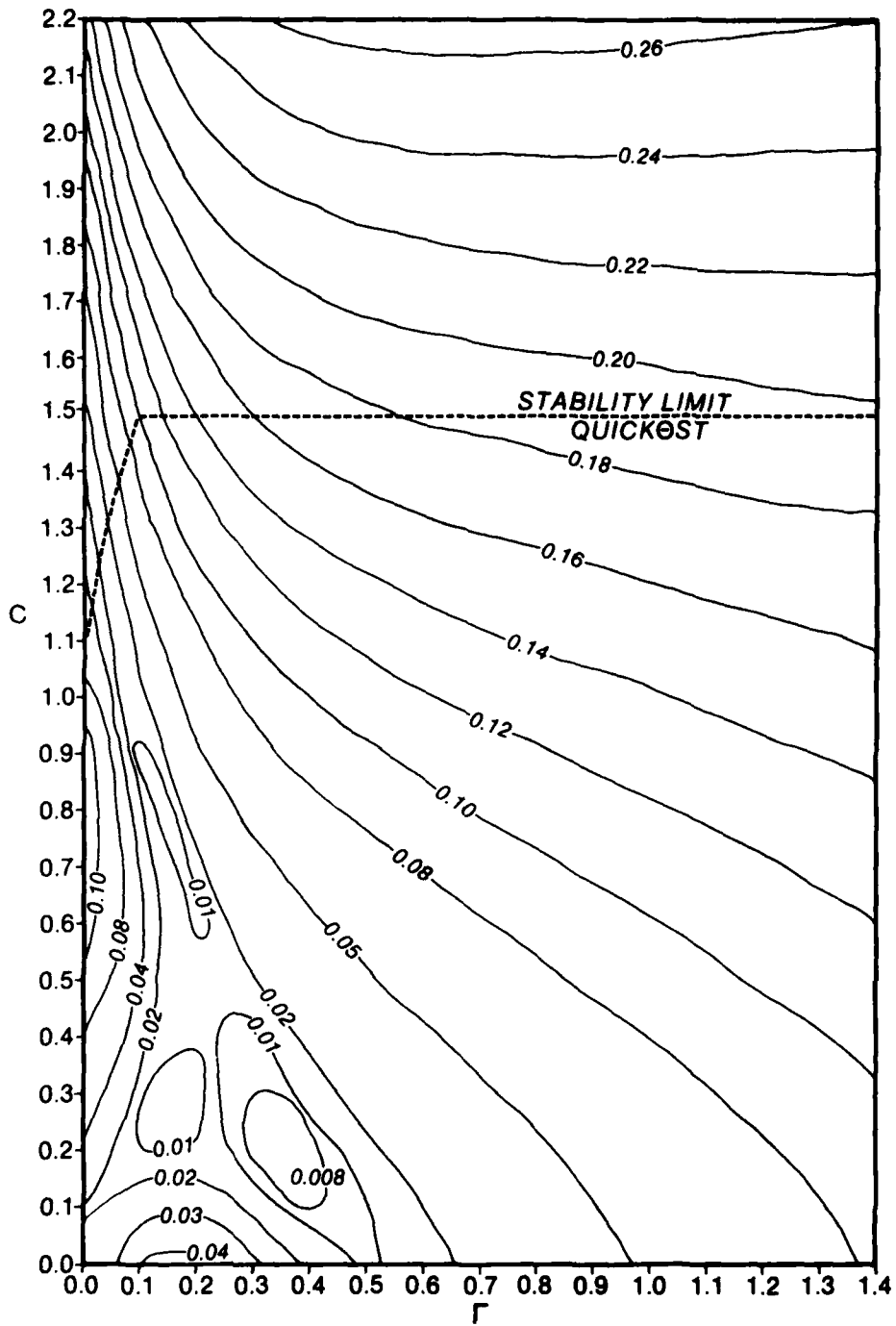Figure 18. Iso-amplitude plot for QUICKθST with stable range also shown

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the extended stable region above C = 1.0 for practical values of
Γ > 0.5 . The phase accuracy for the three schemes generally followed
these same trends.

Propagation tests of QUICKθST

44. The excellent numerical accuracy of the QUICKθST is con-
firmed by the triangle propagation test results depicted in Figure 19.
The discrepancy at the peak is comparable to that produced by the ex-
plicit scheme (Figure 7) and the waviness of the upstream face is due
to phase errors (recall Figure 17). The closeness of numerical results
between the explicit and QUICKθST algorithms is also demonstrated in
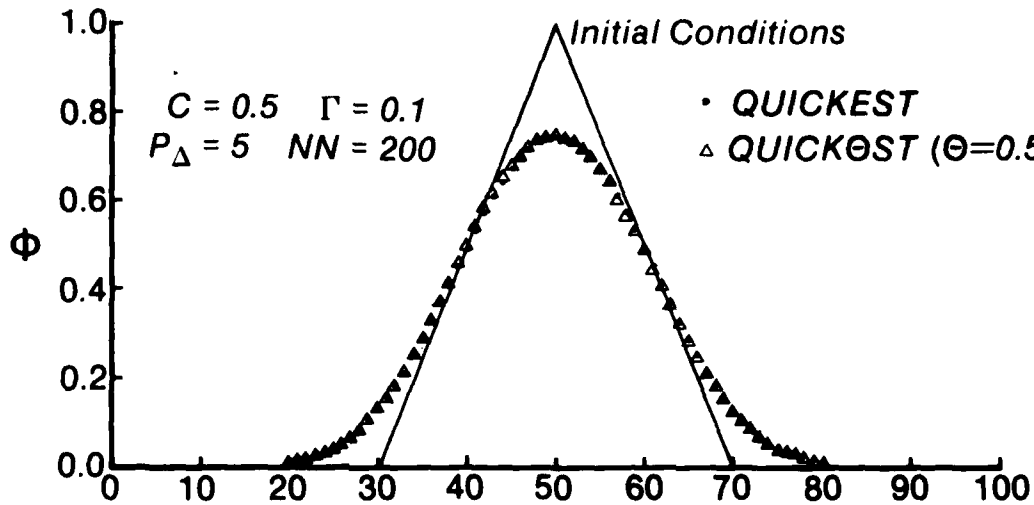Figures 20 and 21 where some physical diffusion (Γ = 0.1) is now present.
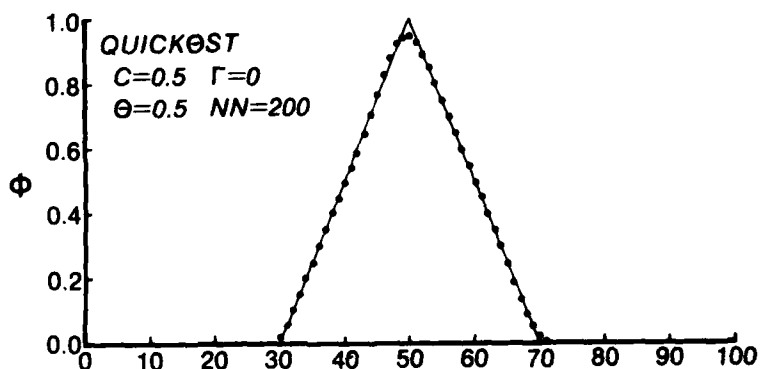
(a) When C=0.5 and after 200 time steps.
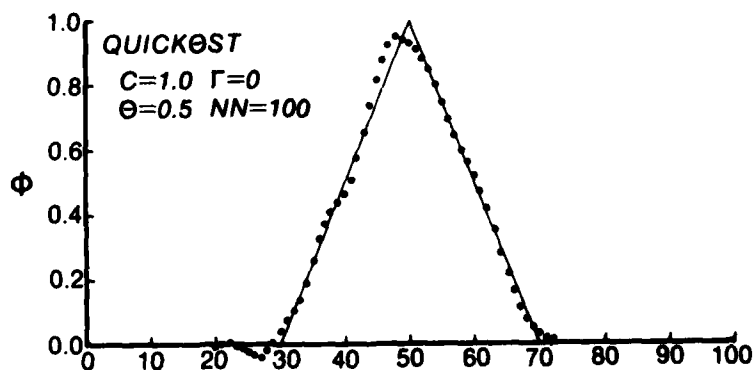
(b) When C=1.0 and after 100 time steps.

Figure 19. Propagation test results for pure advection
case using periodic boundary conditions and QUICKθST
algorithm

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(a) When C=0.5, Γ=0.1, P_Δ=5 and after 200 time steps.
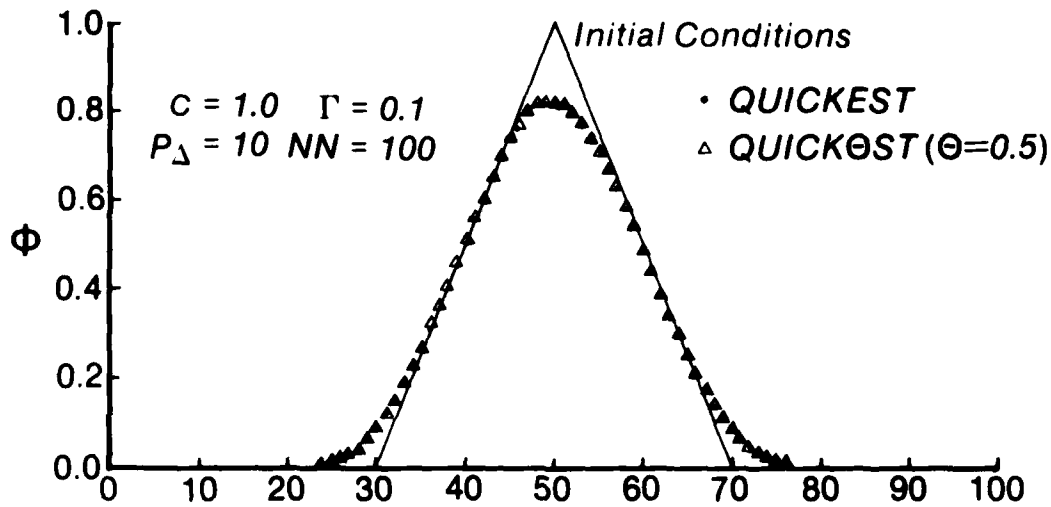
(b) When C=1.0, Γ=0.1, P_Δ=10 and after 100 time steps.

Figure 20. Propagation test results for example with some physical diffusion present (Γ = 0.1) comparing explicit (dots) and implicit (triangles) QUICKθST algorithms

In these examples, only initial conditions are shown.

45. Other propagation tests gave similar results.

Figure 21. Propagation test results for narrow triangle (JW = 2) and
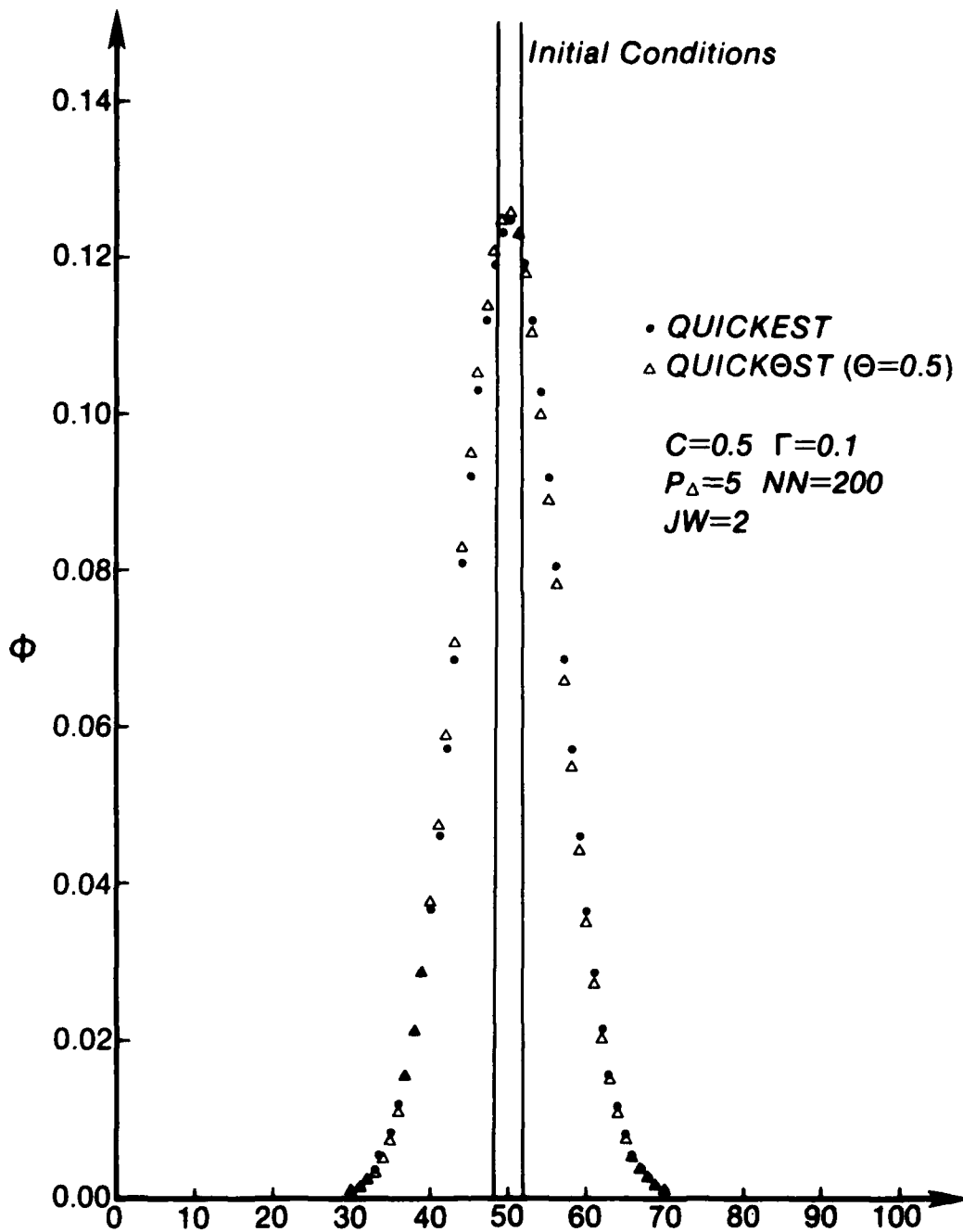physical diffusion (Γ = 0.1) comparing QUICKEST (dots) and QUICKΘST
(triangles) algorithm when C = 0.5 , Γ = 0.1 , P_Δ = 5 after 200
time steps

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PART IV: CONCLUSIONS AND RECOMMENDATIONS

46. The purpose of this project was to develop and study numerical properties of an implicit algorithm consistent with the QUICKEST scheme of Leonard (1979) for the unsteady, one-dimensional transport-diffusion equation. Based upon the results discussed in this report, the following conclusions are drawn and recommendations offered.

Conclusions

47. The explicit algorithm labeled QUICKEST is identical to a forward-time, centered-space scheme with all truncation errors expressed as spatial derivatives and removed through ϕ_{xx} and ϕ_{xxx} terms. The ϕ_{xxx} term is centered upstream and results in a higher order, accurate, upstream difference method.

48. A fully centered, implicit scheme called QUICKθST, as developed herein, is of comparable accuracy to the explicit operator yet extends the stable range in the (Γ, C) plane to essentially below the line, $C = 1.5$ for all Γ .

49. QUICKθST is a stable, accurate, and robust algorithm of considerable engineering usefulness for transport-diffusion computations.

50. Because development of the implicit QUICKθST algorithm has proven to be highly successful, further research on the QUICKθST 2 scheme is not warranted except to learn the reasons for its poor performance.

Recommendations

51. The QUICKθST scheme for one-dimensional flows should be extended to variable grid spacing. Only nomenclature and programming modifications are required.

52. A two-dimensional QUICKθST algorithm should be developed. Use of an alternating-direction implicit (ADI) structure should be considered along with the "double-sweep" solution algorithm.

53. An experimental test program must be devised to fully verify the two-dimensional QUICKθST against existing and new data from both the field and the laboratory.

54. Systems-oriented computer codes and extensive software should be written for ease in application by computational hydraulic engineers.

REFERENCES

Abbott, M. B. 1979. Computational Hydraulics, Pitman, London.

Leonard, B. P. 1979. "A Stable and Accurate Convective Modelling
Procedure Based on Quadratic Upstream Interpolation," Computer Methods
in Applied Mechanics and Engineering, Vol 19, pp 59-98.

Reid, R. O., and Basco, D.R. 1982. "Numerical Convolution for Solution
of Wave Propagation Problems: Filter Scheme Methods," Journal of
Hydraulic Research (to be published).

Roache, P. J. 1977. Computational Fluid Dynamics, Hermosa, Albuquerque,
N. Mex.

APPENDIX A: DERIVATION OF QUICKθST 2

1.   As mentioned in the footnote on page 37, the original expansion
to develop the QUICKθST algorithm discussed in this report was found to
be incorrect (Ross Hall, 19 Oct. 1982, personal communication).   This
Appendix gives the explanation, all corrected equations, and a linear
stability analysis of the results.   This corrected version is dubbed
QUICKθST 2 and is shown to be a far less robust algorithm than the
"chance" algorithm QUICKθST.   For this reason, the original report and
all conclusions were felt to still be valid and the corrected algorithm
QUICKθST 2 relegated to this Appendix.

2.   Consider the schematic operator shown in Figure 16.   The
general two-dimensional Taylor series expansion given in Equation 28 is
correct but the indices should be

$$a = i$$

$$b = n+\theta$$

$$h = \pm\Delta x$$

$$k = +(1-\theta)\Delta t, -\theta\Delta t \tag{A1}$$

This will give, for example, a space difference from n+θ to n+1 (over
+(1-θ)Δt) and from i to i+1 (over +Δx)

$$\phi_{i+1}^{n+1} = \phi_i^{n+\theta} + [\Delta x(\phi_x)_i^{n+\theta} + (1-\theta)\Delta t(\phi_t)_i^{n+\theta}]$$

$$+ \frac{1}{2!}[\Delta x^2(\phi_{xx})_i^{n+\theta} + (1-\theta)^2\Delta t^2(\phi_{tt})_i^{n+\theta} + \underline{2}\Delta x(1-\theta)\Delta t(\phi_{xt})_i^{n+\theta}]$$

$$+ \frac{1}{3!}[\Delta x^3(\phi_{xxx})_i^{n+\theta} + \underline{3}\Delta x^2(1-\theta)\Delta t(\phi_{xxt})_i^{n+\theta}$$

$$+ \underline{3}\Delta x(1-\theta)^2\Delta t^2(\phi_{xtt})_i^{n+\theta} + (1-\theta)^3\Delta t^3(\phi_{ttt})_i^{n+\theta}] \tag{A2}$$

A1

The coefficients underlined in Equation A2, namely the 2 and 3, were inadvertantly left out of this and all other expansions in the original derivation that produced the "chance" algorithm QUICKθST.

    3. The correct expansion gives the following equations.

Corrected Equation 30 (pp 38-39)

(1)   (3)   (7)

$$\left[\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t}\right] + u(1-\theta)\left[\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}\right] + u\theta\left[\frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x}\right]$$

(5)   (9)

$$= K(1-\theta)\left[\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}\right] + K\theta\left[\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}\right]$$

(2)

$$+ \left[\frac{(1-2\theta)\Delta t}{2!}(\phi_{tt}) + \frac{(1-3\theta+3\theta^2)\Delta t^2}{3!}(\phi_{ttt}) + H.O.T.\right]_i^{n+\theta}$$

(4)

$$-u(1-\theta)\left[\theta\Delta t(\phi_{xt}) - \frac{1}{3!}\Delta x^2(\phi_{xxx}) - \frac{3}{3!}\theta^2\Delta t^2(\phi_{xtt}) + H.O.T.\right]_i^{n+\theta}$$

(8)

$$+u\theta\left[(1-\theta)\Delta t(\phi_{xt}) + \frac{1}{3!}\Delta x^2(\phi_{xxx}) + \frac{3}{3!}(1-\theta)^2\Delta t^2(\phi_{xtt}) + H.O.T.\right]_i^{n+\theta}$$

(6)   (10)

$$+K(1-\theta)\left[\frac{6\theta\Delta t}{3!}(\phi_{xxt}) + H.O.T.\right]_i^{n+\theta} - K\theta\left[\frac{6(1-\theta)\Delta t}{3!}(\phi_{xxt}) + H.O.T.\right]_i^{n+\theta} \quad (A3)$$

Corrected Equation 31 (p 39)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u(1-\theta)\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} + u\theta\frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x}$$

$$= K(1-\theta)\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} + K\theta\frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2}$$

(2)

$$+ \left[\frac{u^2\Delta t}{2}(1-2\theta)\right](\phi_{xx})_i^{n+\theta}$$

A2

(2)+(4)+(6)

$$\left[\frac{u\Delta x^2}{6} - \frac{(1-6\theta+6\theta^2)u^3\Delta t^2}{6} - (1-2\theta)uK\Delta t\right](\phi_{xxx})_i^{n+\theta} \tag{A4}$$

where Term (8) + Term (10) $\equiv$ 0

Corrected Coefficients in Equation 32 (p 40)

$$A = \frac{C\theta}{2} - \Gamma\theta - R\theta$$

$$B = 1 + 2\Gamma\theta + 2R\theta$$

$$C_1 = -(\frac{C\theta}{2} + \Gamma\theta + R\theta)$$

$$D = -\frac{C(1-\theta)}{2} + \Gamma(1-\theta) + R(1-\theta) + S$$

$$E = 1 - 2\Gamma(1-\theta) - 2R(1-\theta) - 3S$$

$$F = +\frac{C(1-\theta)}{2} + \Gamma(1-\theta) + R(1-\theta) + 3S$$

$$H = -S \tag{A5}$$

where:

$$R = \frac{C^2}{2}(1-2\theta)$$

$$S = [\frac{C}{6} - \frac{(1-6\theta+6\theta^2)}{6}C^3 - (1-2\theta)C\Gamma] \tag{A5}$$

Corrected Equation 33a (p 40) when C=1.0, Γ=0, θ=0.5, QUICKθST 2

$$\frac{1}{4}\phi_{i+1}^{n+1} + \phi_i^{n+1} - \frac{1}{4}\phi_{i-1}^{n+1} = 0\cdot\phi_{i+1}^n + \frac{1}{4}\phi_i^n + \phi_{i-1}^n - \frac{1}{4}\phi_{i-2}^n \tag{A6}$$

4. A linear stability analysis of QUICKθST 2 using Equation 27 was employed but with coefficients calculated from Equation A5 above. Some results are summarized below for a perfectly centered scheme with θ=0.5.

C	Γ	Remarks
1.0	0	Exact for all α
0.75	0	Stable
0.5	0	Stable
1.0	1.0	Stable

A3

C	Γ	Remarks
1.01	1.0	Unstable
1.5	0	Unstable
2.0	0.5	Unstable

5. The scheme QUICKθST 2 becomes unstable for all Γ when the Courant number exceeds unity which is an unexpected result for an implicit scheme. Using other values of θ (0.4, 0.51, 0.75, 1.0) produced erratic results with a stable region always far smaller than that given by the QUICKθST scheme. We conclude that this algorithm is far less robust and inferior to the QUICKθST algorithm discussed in this report.

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