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COMPUTATIONAL METHODS FOR IDEAL COMPRESSIBLE FLOW

Bram van Leer

INSTITUTE FOR COMPUTER APPLICATIONS IN SCIENCE AND ENGINEERING
NASA Langley Research Center, Hampton, Virginia 23665

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Langley Research Center
Hampton, Virginia 23665

COMPUTATIONAL METHODS FOR IDEAL COMPRESSIBLE FLOW

Bram van Leer[*]

Leiden Observatory, P.O. Box 9513, 2300 RA Leiden, The Netherlands

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[*]Presently at Delft University of Technology, Department of Mathematics and Computer Science, P.O. Box 356, 2600 AJ Delft, The Netherlands

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1. CONSERVATIVE DISSIPATIVE DIFFERENCE SCHEMES

1.1. Introduction: Why Conservative Dissipative Difference Schemes?

In solving problems of gas dynamics it is often permitted to ignore the dissipative processes in the gas, that is, viscous friction and heat conduction. This simplification of the physical picture boils down, mathematically, to a degeneration of the partial differential equations from second-order conservation laws, the Navier-Stokes equations, to first-order conservation laws, the equations of ideal compressible flow (ICF). Even in this approximation there remains a bewildering variety of complicated flow problems.

Particularly notorious are the problems involving such a strong compression of the gas that, in spite of the a priori assumption, dissipation sooner or later dominates the flow, at last in certain regions known as shocks. In a shock the flow quantities undergo a significant change over a distance typical of the dissipative interaction, i.e. the molecular mean free path.

It is, of course, impossible to infer the _structure_ of a shock from the equations of ICF. The concept of ICF traditionally is saved and extended by representing a shock as a flow _discontinuity._

The motion of such an idealized shock may be derived from an integral version of the first-order conservation laws, expressing the particular conservation principle for a finite volume of fluid and a finite lapse of time. Mathematically, this leads to the theory of weak solutions of nonlinar conservation equations. The algebraic equations relating the propagation speed of a discontinutiy to its amplitude are called the jump equations.

Weak solutions are not unique. Shock discontinuties in which friction produces kinetic energy instead of dissipating it, and heat flows from lower

to higher temperatures, are as eligible as their physically realizable counterparts. Clearly a selection criterion must be invoked. We shall accept a weak solution of the first-order conservation equations only if it is the limit solution, for vanishingly small dissipation, of the second-order conservation equations. For gasdynamics this is equivalent to the following requirement: the entropy of the gas, measure of the accumulated effect of dissipation, must not decrease in a shock. This is called the entropy inequality.

Thus, the advantage of lowering the order of the flow equations is partly offset by the need to introduce extra equations and an extra inequality. In consequence, analytic treatment of ICF problems is impossible in all but a few cases. The numerical treatment, however, can be entirely successful. The key to success is the combination of conservation and artificial dissipation.

The idea behind artificial dissipation is that, since in ICF the effect of dissipation is ignored, it may as well be exaggerated. By providing a difference scheme for ICF with sufficiently large dissipative terms it is possible to achieve that shocks, whenever these appear, posses a structure coarse enough to be resolved in the computational grid.

The concept of conservation enters if we make the difference scheme consistent with the integral form, rather than the differential form, of the equations of ICF. The scheme is then said to be "conservative" or to have the "conservation form"; another often-heard description is "finite-volume scheme". It has been shown, in theory and in practice, that, in using a conservative scheme, the numerical stability of a solution containing an admissible shock automatically guarantees the correct motion of the shock. But in order to achieve numerical stability and to select the proper shocks, the scheme indeed has to be dissipative.

1.2. Ḥistory

The first example of a conservative dissipative difference scheme was the first-order-accurate Lax-Friedrichs (LF) scheme, presented and analyzed by Lax (1954). It is the least accurate of its kind and has no practical value today. More influential was its second-order-accurate successor, the Lax-Wendroff (LW) scheme (1960) which still is widely used by aerodynamicists in the two-step form derived by MacCormack (1969).

The survivor among first-order schemes is Godunov's (1959) method based on upwind differencing. The decision which direction is upwind is made on the basis of the speeds of the finite-amplitude waves by which discrete fluid volumes interact. With this strategy, the solution of Riemann's initial-value problem - the shock-tube or diaphragm problem - becomes a building block of the difference scheme. At present we see a rapid expansion of the literature on "approximate Riemann solvers": Roe (1980), Osher (1980), Harten and Lax (1981), Van Leer (1982), Colella (1982); these find their way in first-order as well as higher-order upwind schemes. A review of this subject was given by Harten, Lax and Van Leer (1983); I shall return to it later in the present lecture.

It turns out that the history of conservative dissipative difference schemes is divided more or less by the decades.

During the fifties, first-order-accurate methods were developed and tested. These methods are what now is called "robust" and, schematically speaking, had no other problems than their modest accuracy. Particularly annoying was the numerical diffusion of entropy.

The sixties gave us the second-order-accurate schemes, meaning different kinds of trouble. Numerical oscillations and nonlinear instabilities near shock waves largely spoiled the pleasure of the reduction in artificial dissipation.

During the seventies the design problems of the sixties were gradually solved. For instance, the prevention of numerical oscillations is now well understood. As this knowledge has not been fully absorbed by the ICF community, I have made it the subject of the second lecture.

The eighties have started with an increased interest in explicitly using the physics embedded in the ICF equations for improving the numerical methods. In particular, there is a strong emphasis on upwind differencing. Some modern ideas on how to compute one-dimensional flow are covered by the present lecture; how well these ideas carry over to multi-dimensional flow is investigated in the third lecture.

1.3. A family of second-order finite-volume schemes

I shall illustrate the recent developments in computing one-dimensional ICF on the basis of a family of second-order-accurate difference schemes. The initial-value representation and algorithm structure are the same as in Van Leer (1980); the notation is also the same, except for the present use of a superscript to indicate the time level.

We start with schemes for the scalar linear convection equation

$$q_t + a \, q_x = o, \quad a = \text{constant}, \tag{1}$$

assuming a piecewise linear initial-value distribution

$$q(x,t^n) = q_i^n + \frac{\delta_i q^n}{\Delta x} (x - x_i), \quad x_{i-\frac{1}{2}} \equiv x_i - \tfrac{1}{2}\Delta x < x < x_{i+\frac{1}{2}}, \tag{2}$$

as in Van Leer (1980), Fig. 4. The gradient is computed by averaging the

numerical gradient values in the neighborhood of x_i:

$$\delta_i q^n = \tfrac{1}{2}(1-\kappa) \, \Delta_{i-\frac{1}{2}} q^n + \tfrac{1}{2}(1+\kappa) \, \Delta_{i+\frac{1}{2}} q^n .$$
(3)

For the moment, the weight κ is assumed to be independent of q. The three possible values of κ most frequently met are

$$\kappa = \text{sgn } a \equiv s, \ 0 \text{ and } -s ,$$
(4)

leading to the LW scheme, Fromm's (1967) scheme and Moretti's (1979) λ -scheme, respectively.

The evolution in one time-step of the initial-value distribution discretized as above is now computed exactly, namely, by shifting the distribution over a distance $a\Delta t$. Averaging over the finite volumes then yields the updated values q_i^{n+1} , from which the gradient in each volume can again be determined.

The LW scheme involves only the downwind value of the gradient of q^n. Shifting the inital-value distribution brings upwind information to x_i, so that the LW scheme ultimately is independent of the sign of a. The LW scheme is a so-called central-difference scheme and involves q_{i-1}^n, q_i^n, and q_{i+1}^n to find q_i^{n+1} . It is stable for

$$\|\sigma\| \leqslant 1,$$
(5.1)

where

$$|\sigma| = a\Delta t/\Delta x$$
(5.2)

is the Courant-Friedrichs-Lewy (CFL) number, and produces a predominantly negative phase error (see Fromm (1967)).

Fromm's scheme is upwind biased, involves q_{i-2s}, q_{i-s}, q_i and q_{i+s}, and

has a zero phase error at $\sigma = s/2$ for all frequencies. Its stability domain is given by (5.1).

The λ-scheme, involving only the upwind value of the gradient of q^n, remains fully one-sided; the values q_{i-2s}, q_{i-s} and q_i are used to compute q_i^{n+1}.

Its stability condition is

$$|\sigma| \leqslant 2 , \tag{6}$$

but in practice we have to put up with (5.1), in order not to complicate the preservation of monotonicity. Under (5.1) the phase error of the λ-scheme is predominantly positive (see Fromm (1967)).

1.4. From convection to ICF

In order to convert the above difference schemes for a single linear convection equation into schemes for the hyperbolic system of the nonlinear conservation laws of ICF, we must regard equation (1) as one of the characteristic (diagonalized) equations, q as a characteristic state quantity and a as a characteristic speed; see Van Leer (1980). Since a now depends on q, so does κ, and it suddenly appears impractical (although feasible) to use any other value than $\kappa = 0$. This leads to the following observation:

In upwind-biased schemes the discretized initial-value distribution is independent of the direction in which the various physical signals propagate; see Van Leer (1977).

Restricting ourselves to Fromm's scheme, we follow the recipe from [24] for advancing in time (the approach by Van Leer (1979) is different). We first update the distribution in each volume over a half step in time,

without regard to the neighboring volumes, with a central-difference scheme. For the characteristic quantities (other state quantities may be used) this boils down to

$$q_i^{n+\frac{1}{2}} = q_i^n - \tfrac{1}{2}\sigma_i^n \cdot \delta_i q^n, \qquad (7.1)$$

$$\delta_i q^{n+\frac{1}{2}} = \delta_i q^n , \qquad (7.2)$$

with sufficient accuracy.

Subsequently, time-centered values are obtained on the upwind side of each interface. For ICF, described by the system of conservation laws

$$w_t + [f(w)]_x = 0, \qquad (8)$$

this means we must compute the complete states w_L and w_R on the left and right side of each interface and solve the local Riemann problem, exactly or approximately, to find out what the upwind components are. In formula:

$$q_{(i\pm\frac{1}{2})\mp}^{n+\frac{1}{2}} = q_i^{n+\frac{1}{2}} \pm \tfrac{1}{2}\delta_i q^n , \qquad (9.1)$$

$$w_{(i\pm\frac{1}{2})\mp}^{n+\frac{1}{2}} = w(q_{(i\pm\frac{1}{2})\mp}) , \qquad (9.2)$$

$$F_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \Phi(w_{(i+\frac{1}{2})-}^{n+\frac{1}{2}} , w_{(i+\frac{1}{2})+}^{n+\frac{1}{2}}) ; \qquad (9.3)$$

here $\Phi(w_L, w_R)$ is the flux resulting at an interface after resolution of the initial discontinuity and F is the numerical flux vector used to approximately integrate the system (8) over one time step and one finite volume:

$$\frac{w_i^{n+1} - w_i^n}{\Delta t} + \frac{F_{i+\frac{1}{2}}^{n+\frac{1}{2}} - F_{i-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x} = 0 . \qquad (10)$$

Note that twice in this second-order scheme there is an exchange of information between neighboring volumes.

The first exchange, finite-differencing of q_i at t^n, is purely numerical – initial-value interpolation – and involves no physics. We may at this stage use any complete set of state quantities; the choice of characteristic quantities is imperative only near boundaries and advisable near discontinuities.

The second exchange, solving the Riemann problem defined by $w_{(i+\frac{1}{2})}^-$ and $w_{(i+\frac{1}{2})+}$, is purely physical: interaction through waves. Simplifying the solution of the Riemann problem, while desirable for numerical reasons, is a matter of simplifying the physics of the wave interactions.

1.5. Approximate Riemann solvers

I shall discuss two distinct approximate solvers of Riemann's problem: the one by Roe (1980), based on linear waves, and the one by Van Leer (1982), based on material transport.

Roe solves the Riemann problem defined by the initial values

$$
w = \left\{ \begin{array}{ll} w_L & x < 0 \ , \\ w_R & x > 0 \ , \end{array} \right. \tag{11}
$$

by solving it for a linearization of Eq. (10):

$$
w_t + \hat{A}\,(w_L,\, w_R)\, w_x = 0 \ , \tag{12}
$$

where $\hat{A}(w_L, w_R)$ is some average of

$$A(w) \equiv df(w)/dw \qquad (13)$$

over the interval (w_L, w_R).

Mathematically it is clear that

$$\hat{A}(w_L, w_R) = A(\frac{w_L + w_R}{2}) + O((w_R - w_L)^2) , \qquad (14)$$

which is fine for weak waves. Roe demands that the solution also be exact if there is only one wave with a nonzero amplitude; this wave, however, maybe arbitrarily strong. This can be achieved only by chosing $\hat{A}$ such that

$$\hat{A}(w_L, w_R) \cdot (w_R - w_L) = f(w_R) - f(w_L) , \qquad (15)$$

the discrete analogue of (13). If w_R and w_L can be connected by a single discontinuity with speed U, the jumps in w and f are connected by the jump equation

$$U(w_R - w_L) = f(w_R) - f(w_L). \qquad (16)$$

Upon comparison of (15) and (16) it follows that $w_R - w_L$ is an eigenvector of $\hat{A}$, and U the corresponding eigenvalue.

Harten (1981) has shown for hyperbolic systems (8) admitting an entropy condition, that the mean value

$$\hat{A}(w_L, w_R) = \int_0^1 A(w_L + \theta(w_R - w_L)) d\theta \qquad (17)$$

not only satisfies (15) but also has a complete set of real eigenvectors and eigenvalues, making Eq. (12) hyperbolic under all circumstance.

Roe (1981) has indicated an algebraic procedure to construct matrices $\hat{A}(w_L, w_R)$ of the form $\hat{A}(\hat{w})$ where $\hat{w}$ is some average of w_L and w_R. His arguments bear heavily on the specific homogeniety properties of the conservation laws involved.

Once $\hat{A}$ has been found, it is split in its positive and negative parts $\hat{A}^+$ and $\hat{A}^-$; positive and negative refer to the eigenvalues of the matrix. Correspondingly we may split $\Delta f \equiv f(w_R) - f(w_L)$ in

$$(\Delta f)^+ = \hat{A}^+ (w_R - w_L) , \qquad\qquad (18.1)$$

$$(\Delta f)^- = \hat{A}^- (w_R - w_L) , \qquad\qquad (18.2)$$

the changes of the flux across the forward moving and backward moving waves, respectively. This is called flux-difference splitting.

It is easy to see that the flux $\Phi(w_L, w_R)$ needed in Eq. (9.3) equals

$$\Phi(w_L, w_R) = f(w_L) + (\Delta f)^- \qquad\qquad (19.1)$$

$$= f(w_R) - (\Delta f)^+ ; \qquad\qquad (19.2)$$

see also ApI, Fig. 8.

A word of caution: the jump condition (16) does not imply the entropy condition: w_L and w_R may be exchanged. Likewise, if

$$\hat{A}(w_L, w_R) = \hat{A}(w_R, w_L) , \qquad\qquad (20)$$

the scheme incorporating $\hat{A}$ can not recognize inadmissible shocks and may not destroy these. Some asymmetry must therefore be introduced in the dependence of $\hat{A}$ on w_L and w_R; see Harten and Lax (1981).

An alternative to (18) is to split the flux itself:

$$f(w) = f^+(w) + f^-(w) \; ; \qquad\qquad\qquad (21)$$

$f^+(w)$ and $f^-(w)$ may be called the forward and the backward flux, respectively. In the review by Harten, Lax and Van Leer (1983) it is demonstrated that this kind of splitting follows from interpreting the conservation laws (8) as moments of the collisionless Boltzmann equation, using a numerically convenient particle-velocity distribution.

Van Leer (1982) shows how to achieve a splitting like (21) for the flux in the Euler equations. Care must be taken to ensure that $f^+(w)$ and $f^-(w)$ are continuously differentiable functions of w, so that Eq. (8) can be consistently approximated. In contrast, $\hat{A}^+(w_L, w_R)$ and $\hat{A}^-(w_L, w_R)$ in the flux-difference splitting (18) just have to be continuous. In any case, second-order terms with split fluxes or split flux-differences must be avoided; see Mulder and Van Leer (1983).

1.6 Alternative ways of time-stepping

If temporal accuracy is not needed, for instance, in marching toward a steady state, we retain from the scheme from Sec. 1.4 only the steps relating to the approximation of f_x. Following Jameson et al. (1981) we may advance in time with an m-step Runge-Kutta algorithm:

$$w_i^{(0)} = w_i^n$$

$$w_i^{(k)} = w_i^n - \frac{\alpha^{(k)}}{k!} \Delta t \; \Delta_i F^{(k-1)}/\Delta x, \quad k=1,..,m,$$

$$\alpha^{(m)} = 1 \; ,$$

$$w_i^{(m)} = w_i^{n+1} \; . \tag{22}$$

Once a steady state is achieved it is independent of Δt. The same steady state would be found with the two-step scheme from Sec. 1.4, in the limit of $\Delta t \to 0$.

Unfortunately, the stability condition associated with upwind-biased spatial-differencing operators is rather restrictive, due to the sizable negative real part of the eigenvalues of such operators. This is illustrated in Figure 1 (taken from work done in collaboration with E. Turkel (1982)), for the combination of Fromm's space-differencing and fourth-order four-step Ringe-Kutta time-stepping $(\alpha^{(k)} = 1, \; k = 1,2,3,4)$. The stability conditon after four steps is a meagre

$$|\sigma| \lesssim 1.4 \; ; \tag{23.1}$$

changing the coefficients $a^{(3)}$ and $\alpha^{(4)}$ improves this up to

$$|\sigma| \lesssim 1.9 \; . \tag{23.2}$$

In contrast, the central-differencing operator of the LW scheme, which has purely imaginary eigenvalues, leads to a stability condition

$$|\sigma| \lesssim 2.8 \; , \tag{23.3}$$

see Jameson et al. (1981). We conclude that upwind differencing is not efficient in combination with Runge-Kutta time-stepping.

Another possibility is to use implicit time stepping, such as the "backward Euler" or "implicit Euler" method. In practice the implicit difference scheme must be linearized in time to make inversion possible. The

linearization is only feasible if the numerical flux-function F is differentiable with respect to its arguments. This requirement favors the use of flux-vector splitting; see Mulder and Van Leer (1983).

2. THE RECOGNITION AND REPRESENTATION OF DISCONTINUITIES

2.1. Monotone initial-value interpolation

The formula (3) for $\delta_i q^n$ is based on the assumption that the gradient of w varies smoothly between x_{i-1} and x_{i+1}. If w or its first derivative is discontinuous in this interval, the value of δ thus computed is meaningless and, when used, may give rise to numerical oscillations. The sight of a shock with numerical oscillations is well known and needs no illustration here.

A local discontinuity in w or w_x may be recognized, in a sequence of mesh-refinements, by a local extremum of $\Delta_{i+\frac{1}{2}} w / \Delta_{i-\frac{1}{2}} w$ that goes to infinity or to a finite value $\neq 1$. The only place in a smooth solution where this behaviour is also seen is at an extremum.

It has been demonstrated by Van Leer (1972, 1974, 1977) that meaningful values of δ are obtained under the extra constraint of monotonicity. For a linear convection equation it says that the updated discrete distribution must be monotone if the discrete initial-value distribution is monotone; this of course, is true for the exact solution. Satisfying this condition turns out to simply be a matter of monotonicly interpolating the initial values inside volumes.

To fix our thoughts, let $q_{i-1}^n \leqslant q_i^n \leqslant q_{i+1}^n$ and $0 \leqslant \sigma \leqslant 1$; We shall use the abbreviations $\Delta_- \equiv \Delta_{i-\frac{1}{2}} q^n$, $\Delta_+ = \Delta_{i+\frac{1}{2}} q^n$, $\delta_i q^n \equiv \delta$. It is easily seen that, for the preservation of monotonicity at t^{n+1}, we must limit δ as follows:

$$\delta \leq \{ \begin{array}{l} \dfrac{2}{1-\sigma} \Delta_+ \quad \text{(no overshoot in } x_{i+1} \text{ for } \sigma \overset{\sim}{\sim} 0) \\[2mm] \dfrac{2}{\sigma} \Delta_- \quad \text{(no overshoot in } x_i \text{ for } \sigma \overset{\sim}{\sim} 1) \end{array} \qquad (34)$$

Note that, regardless of the value of σ, δ must vanish if Δ_+ or Δ_- vanishes. Taking the minimum of condition (34) over all values of σ, we arrive at

$$\delta \leq \min \ (2\Delta_-, \ 2\Delta_+). \qquad (35)$$

With δ within these bounds, the initial values (2) inside volume i will not go beyond the neighboring zone averages; see Van Leer (1980).

For the three schemes of Sec. 1.3, (35) means that no limiting is necessary if

$$\text{(LW)} \qquad 0 \leq \Delta_+/\Delta_- \leq 2 \ , \qquad (36.1)$$

$$\text{(Fromm)} \quad \frac{1}{3} \leq \Delta_+/\Delta_- \leq 3 \quad , \qquad (36.2)$$

$$\text{(}\lambda\text{)} \qquad \tfrac{1}{2} \leq \Delta_+/\Delta_- \leq \infty \quad . \qquad (36.3)$$

Using

$$S_1 = (\Delta_+ - \Delta_-)/(\Delta_+ + \Delta_-) \overset{\sim}{\sim} \frac{\Delta x}{2} (\ln w_x)_x \qquad (37)$$

as a "smoothness monitor" (the logarithmic second derivative is a measure of curvature), we can write (36) as

$$\text{(LW)} \qquad -1 \leq S_1 \leq \frac{1}{3} \ , \qquad (38.1)$$

$$\text{(Fromm)} \quad -\tfrac{1}{2} \leq S_1 \leq \tfrac{1}{2} \ , \qquad (38.2)$$

$$(\lambda) \qquad -\frac{1}{3} \leqslant S_1 \leqslant 1 \; . \tag{38.3}$$

For the Fromm scheme, the permitted range (36.2) or (38.2) remains the same when the sign of σ is flipped; this is not true for the ranges associated with the other schemes. Hence, the initial-value dicretization for Fromm's scheme remains independent of the physics.

2.2. Limiters, switches and artificial dissipation

Eq. (35) can be satisfied by limiting δ:

$$\delta_{lim} = \min \; (2\Delta_-, \; \delta, \; 2\Delta_+) \; , \tag{39}$$

but a smoother dependence on Δ_+/Δ_- is preferable. Harmful effects of clipping caused by suddenly acting limiters like (39) are described by Van Leer (1977), Woodward and Colella (1982) and Van Albada et al. (1982).

In the latter paper a smooth limiter for Fromm's scheme was described:

$$\delta_{lim} = \frac{(\Delta_+^2 + \varepsilon^2)\Delta_- + (\Delta_-^2 + \varepsilon^2)\Delta_+}{\Delta_+^2 + \Delta_-^2 + 2\varepsilon^2} \tag{40.1}$$

$$= \frac{2\Delta_+\Delta_- + 2\varepsilon^2}{\Delta_+^2 + \Delta_-^2 + 2\varepsilon^2} \cdot \frac{\Delta_+ + \Delta_-}{2} \tag{40.2}$$

$$= \left\{ 1 - \frac{(\Delta_+ - \Delta_-)^2}{\Delta_+^2 + \Delta_-^2 + 2\varepsilon^2} \right\} \cdot \frac{\Delta_+ + \Delta_-}{2} \; ; \tag{40.3}$$

here ε^2 is a small threshold that also prevents zerodivide. The treshold can be chosen such that the limiting effect disappears in the neighborhood of a smooth extremum, that is, when Δ_+ and Δ_- have values $\sim (\Delta x)^2$.

Clearly, $\varepsilon^2 \sim (\Delta x)^3$ will do.

Eq. (40.1) shows that $\delta_{\lim}$ is a weighted average of Δ_+ and Δ_- , biased toward the smaller of the two. In the limit of $\Delta_+/\Delta_- = \infty$ or 0 , the average equals the smaller value. Eqs. (40.2) and (40.3) show that $\delta_{\lim}$ equals its unlimited value (3) multiplied by a switch factor; this factor falls about

$$S_2 \overset{\sim}{\sim} \tfrac{1}{2}(\Delta x)^2 \ (\ln w_x)_x\}^2 \qquad\qquad (40.4)$$

short of unity in a smooth solution. The appearance of the logarithmic second derivative is no surprise.

A tighter fit to (39) is

$$\delta_{\lim} = \frac{(2\Delta_+^2 + \varepsilon^2)\Delta_- + (2\Delta_-^2 + \varepsilon^2)\Delta_+}{\Delta_+^2 + 2|\Delta_+\Delta_-| + \Delta_-^2 + 2\varepsilon^2} \qquad\qquad (41)$$

which tends toward twice the smaller of Δ_- and Δ_+ , in the limit of $\Delta_+/\Delta_- = \infty$ or 0.

Eqs. (40) and (41) also limit the value of δ if the signs of Δ_+ and Δ_- are different, that is, if the initial-value sequence is not monotone. The numerical experiments of Mulder and Van Leer (1983) suggest that (40) gives a cleaner representation of the solution near a steady shock than (41).

The effect of the switch factor in (40) on the scheme can be interpreted in several ways. According to (40.2) the switch turns off the nominal gradient in a zone; since it is the gradient that leads to second-order accuracy, the switch can be said to turn off the second-order term of the scheme. Symbolicly (ignoring the conservation form):

$$(L_2)_{lim} = L_2 + S_2 (L_1 - L_2), \qquad\qquad (42.1)$$

here L_2 and L_1 are the second-order operator and embedded first-order operator. Since L_1-L_2 is predominantly a dissipative term, S_2 must be an artificial-dissipation coefficient.

Writing (42.1) as

$$(L_2)_{lim} = (1 - S_2) L_2 + S_2 L_1, \qquad\qquad (42.2)$$

reveals that $(L_2)_{lim}$ symbolizes a so-called hybrid scheme, see Harten (1978). Writing (42.1) as

$$(L_2)_{lim} = L_1 + (1 - S_2)(L_2 - L_1) \qquad\qquad (42.3)$$

reminds us of the Flux-Corrected Transport (FCT) methods of Boris and Book (1973), where a first-order result is improved by adding a limited second-order term. These, however, are the methods mentioned earlier that show the disastrous clipping effect.

2.3 Nonlinear case

The analysis in 2.1 shows that for a linear convection equation the monotonicity of the numerical solution can be preserved by monotone interpolation of the solution inside each volume. This recipe works surprisingly well for nonlinear convection and seldom needs adjustments; see, however, Woodward and Colella (1982), Colella and Woodward (1982). For single nonlinear conservation laws it can be made exact; see Harten (1982).

What do shock profiles, computed with monotonicity preserving schemes, look like? To answer this question an example of shock propagation by three upwind-biased schemes based on monotone initial-value interpolation is given in Figure 2, taken from Woodward (1980).

2.4 Related subjects

So far we have only discussed the role of the initial-value representation in preserving monotonicity. Obviously the choice of the time-stepping algorithm will influence the numerical results. The sharpness of steady shocks, for instance, depends on the Riemann solver used, although the differences among second-order schemes are much less important than among first-order schemes; see e.g. Van Leer (1981). (This subject will be reviewed in a forthcoming paper by Enquist, Osher, Roe, and Van Leer (1983)).

Discontinuities that have spread too much, in particular contact discontinuities, may be steepened by applying Harten's (1977) artificial compression method (ACM).

It is possible to use a smoothness monitor for other purposes than to limit gradient values. Some applications are: to indicate where the grid should be refined or moved, and where shock-fitting or shock-recovery should be carried out; for the latter subject see Morton (1982).

3. MULTI-DIMENSIONAL METHODS

3.1 Multi-dimensional convection

In order to illustrate how the one-dimensional schemes of Section 2 can

be applied in multi-dimensional problems, I shall discuss two first-order schemes for convection in two dimensions.

Godunov's one-dimensional scheme is what we get if, in the schemes studied previously, δq is always set equal to zero. In other words, the initial values in each volume are chosen to be uniform, which accounts for the loss of the second-order accuracy. The Lax-Friedrichs scheme also uses uniform initial values in each volume but the grid is staggered in time. I shall start with the latter.

The convection equation to be approximated is

$$q_t + aq_x + bq_y = 0, \quad a > 0, \ b > 0. \tag{43}$$

For convenience the points (x_i, y_j), (x_{i-1}, y_j), (x_i, y_{j-1}) and (x_{i-1}, y_{j-1}), and the volumes centered at these points are indicated by A, B, C and D, respectively; the center $(x_{i-\frac{1}{2}}, y_{j-\frac{1}{2}})$ of the staggered volume is indicated by M. This is shown in Figure 3a.

After moving the piecewise-uniform distribution with a velocity (a,b) over a time interval Δt we find, by weighting q according to area (see Figure 3b):

$$q_M^{n+1} = (\tfrac{1}{2} - \sigma_x)(\tfrac{1}{2} - \sigma_y)q_A^n + (\tfrac{1}{2} + \sigma_x)(\tfrac{1}{2} - \sigma_y)q_B^n +$$

$$+ (\tfrac{1}{2} - \sigma_x)(\tfrac{1}{2} + \sigma_y)q_C^n + (\tfrac{1}{2} + \sigma_x)(\tfrac{1}{2} + \sigma_y)q_D^n, \quad \sigma_x, \sigma_y \leqslant \tfrac{1}{2}. \tag{44.1}$$

For comparison with Eq. (10) we may rewrite this as

$$q_M^{n+1} = \tfrac{1}{4}(q_A^n + q_B^n + q_C^n + q_D^n)$$

$$- \sigma_x [\{(\tfrac{1}{2}-\tfrac{1}{2}\sigma_y)q_A^n + (\tfrac{1}{2}+\tfrac{1}{2}\sigma_y)q_C^n\}-\{(\tfrac{1}{2}-\tfrac{1}{2}\sigma_y)q_B^n + (\tfrac{1}{2}+\tfrac{1}{2}\sigma_y)q_D^n\}]$$

$$- \sigma_y [\{(\tfrac{1}{2}-\tfrac{1}{2}\sigma_x)q_A^n + (\tfrac{1}{2}+\tfrac{1}{2}\sigma_x)q_B^n\}-\{(\tfrac{1}{2}-\tfrac{1}{2}\sigma_x)q_C^n + (\tfrac{1}{2}+\tfrac{1}{2}\sigma_x)q_D^n\}]$$

$$\equiv q_M^n - \sigma_x(q_E^{n+\frac{1}{2}} - q_W^{n+\frac{1}{2}}) - \sigma_y(q_N^{n+\frac{1}{2}} - q_S^{n+\frac{1}{2}}). \qquad (44.2)$$

Here $q_E^{n+\frac{1}{2}}$ is the time-average of the space average of q on the East side (AC) of volume M; the other averages are defined similarly. This formula differs from the version given orignally by Lax (1954), where the fluxes through the sides of volume M are not centered in time. This removes the cross-difference term $\sigma_x\sigma_y(q_A^n - q_B^n - q_C^n + q_D^n)$ from the scheme and reduces the scheme's stability domain.

Scheme (44) can be written as the product of two one-dimensional LF schemes:

$$q_{i-\frac{1}{2}\,j-\frac{1}{2}}^{n+1} = [\tfrac{1}{2}(1+T_y^{-1}) - \sigma_y(1-T_y^{-1})][\tfrac{1}{2}(1+T_x^{-1}) - \sigma_x(1-T_x^{-1})]q_{ij}^n$$

$$\equiv L_y^{LF}(\Delta t)\, L_x^{LF}(\Delta t)q_{ij}^n, \qquad (45)$$

where T_x and T_y denote a forward translation by one volume in the x- and y-direction. Hence, the method of fractional time-steps or time-splitting is exact for the linear LF scheme.

Godunov's scheme, illustrated in Figure 4, can be written as

$$q_A^{n+1} = (1-\sigma_x)(1-\sigma_y)q_A^n + \sigma_x(1-\sigma_y)q_B^n + \sigma_y(1-\sigma_x)q_C^n + \sigma_x\sigma_y q_D^n \qquad (46.1)$$

or

$$q_A^{n+1} = q_A^n - \sigma_x[\{(1-\tfrac{1}{2}\sigma_y)q_A^n+\tfrac{1}{2}\sigma_y q_C^n\}-\{(1-\tfrac{1}{2}\sigma_y)q_B^n+\tfrac{1}{2}\sigma_y q_D^n\}]$$

$$- \sigma_y [\{ (1-\tfrac{1}{2}\sigma_x) q_A^n + \tfrac{1}{2} \sigma_x q_B^n \} - \{ (1-\tfrac{1}{2}\sigma_x) q_C^n + \tfrac{1}{2}\sigma_x q_D^n \}]$$

$$\equiv q_A^n - \sigma_x (q_E^{n+\frac{1}{2}} - q_W^{n+\frac{1}{2}}) - \sigma_y (q_N^{n+\frac{1}{2}} - q_S^{n+\frac{1}{2}}), \qquad (46.2)$$

where E, W, N and S now refer to the sides of volume A. Again the proper cross-difference term is included and exact factorization is possible:

$$q_{ij}^{n+1} = \{ (1-\sigma_y(1-T_y^{-1})) \} \; \{ 1-\sigma_x(1-T_x^{-1}) \} q_{ij}^n$$

$$\equiv L_y^G(\Delta t) \; L_x^G(\Delta t) \; q_{ij}^n \; . \qquad (46)$$

3.2 From convection to ICF

The LF scheme can be exactly implemented for a nonlinear system of conservation laws

$$w_t + [f(w)]_x + [g(w)]_y = 0 \; . \qquad (47)$$

The flux $aq_E^{n+\frac{1}{2}}$ through the East side of M is changed into $F_E^{n+\frac{1}{2}}$, with

$$F_E^{n+\frac{1}{2}} = \frac{1}{\Delta t \Delta y} \int_{t^n}^{t^{n+1}} \int_C^A f(w_{AC}^n(t,y)) \; dy \; dt \; , \qquad (48)$$

where $w_{AC}^n (t,y)$ is the time-dependent solution of the one-dimensional Riemann problem on the line CA with initial values at t^n. The other fluxes are obtained similarly.

An useful approximation of (48) results if we first average w:

$$w_E^{n+\frac{1}{2}} = \frac{1}{\Delta t \Delta y} \int_{t^n}^{t^{n+1}} \int_C^A w_{AC}^n(t,y) \, dy \, dt$$

$$= \tfrac{1}{2}(w_A^n + w_C^n) - \frac{\Delta t}{2\Delta x}(g_A^n - g_C^n) \, , \tag{49}$$

and then adopt

$$F_E^{n+\frac{1}{2}} = f(w_E^{n+\frac{1}{2}}) \, , \tag{50}$$

which differs $O((\Delta x)^2)$ from (48). Note that, owing to conservation, the computation of the average $w_E^{n+\frac{1}{2}}$ does not require knowledge of the detailed Riemann solution.

Eq. (49) is, of course, the one-dimensional LF scheme for flow along the line CA. This inspires the following implementation of the LF scheme for Eq. (47).

$$\widetilde{w}_{i j-\frac{1}{2}}^{n+\frac{1}{2}} = L_y^{LF}(\frac{\Delta t}{2}) \, w_{ij}^n \tag{51.1}$$

$$\widetilde{\widetilde{w}}_{i-\frac{1}{2} j}^{n+\frac{1}{2}} = L_x^{LF}(\frac{\Delta t}{2}) \, w_{ij}^n \tag{51.2}$$

$$w_{i-\frac{1}{2} j-\frac{1}{2}}^{n+1} = \frac{1}{4}(w_{ij}^n + w_{i-1j}^n + w_{ij-1}^n + w_{i-1j-1}^n)$$

$$- \frac{\Delta t}{\Delta x}(\widetilde{f}_{i j-\frac{1}{2}}^{n+\frac{1}{2}} - \widetilde{f}_{i-1 j-\frac{1}{2}}^{n+\frac{1}{2}}) - \frac{\Delta t}{\Delta y}(\widetilde{g}_{i-\frac{1}{2} j}^{n+\frac{1}{2}} - \widetilde{g}_{i-\frac{1}{2} j-1}^{n+\frac{1}{2}}) \tag{51.3}$$

This version is symmetric in x and y, just as the time-splitting suggested by Strang (1968) for two-dimensional operators:

$$L_{2D}(\Delta t) = \tfrac{1}{2}\{L_x(\Delta t)L_y(\Delta t) + L_y(\Delta t)L_x(\Delta t)\} \, , \tag{52.1}$$

It must be said, however, that computational fluid dynamists almost exclusively use pure product operators like (45). To reduce the asymmetry betwen x and y, the sequence $L_y L_x$ is alternated with $L_y L_x$:

$$L_2(2\Delta t) = L_x(\Delta t)L_y(\Delta t)L_y(\Delta t)L_x(\Delta t) \ . \qquad (52.2)$$

The exact formulation of Godunov's scheme for Eq. (47) requires knowledge of the solution of Riemann's problem in two dimensions, with initial values uniform in each quadrant. This solution is only known for a single conservation law and was obtained by Wagner (1980). In the same way as (51) is derived from (44b), we may derive from (46.2) an approximation to Godunov's scheme based entirely on the solution of one-dimensional Riemann problems:

$$\widetilde{w}_{ij}^{n+\frac{1}{2}} = L_y^G(\frac{\Delta t}{2})w_{ij}^n \ , \qquad (53.1)$$

$$\widetilde{w}_{ij}^{n+\frac{1}{2}} = L_x^G(\frac{\Delta t}{2})w_{ij}^n \ , \qquad (53.2)$$

$$w_{ij}^{n+1} = w_{ij}^n - \frac{\Delta t}{\Delta x}(\widetilde{F}_{i+\frac{1}{2}j}^{n+\frac{1}{2}} - \widetilde{F}_{i-\frac{1}{2}j}^{n+\frac{1}{2}}) - \frac{\Delta t}{\Delta y}(\widetilde{G}_{ij+\frac{1}{2}}^{n+\frac{1}{2}} - \widetilde{G}_{ij-\frac{1}{2}}^{n+\frac{1}{2}}) \ . \qquad (53.3)$$

Here

$$\widetilde{F}_{i+\frac{1}{2}j}^{n+\frac{1}{2}} \equiv \Phi(\widetilde{w}_{ij}^{n+\frac{1}{2}}, \widetilde{w}_{i+1j}^{n+\frac{1}{2}}) \ , \quad \widetilde{G}_{ij+\frac{1}{2}}^{n+\frac{1}{2}} \equiv \Phi(\widetilde{w}_{ij}^{n+\frac{1}{2}}, \widetilde{w}_{ij+1}^{n+\frac{1}{2}}) \ , \qquad (53.4)$$

with the Riemann flux $\Phi(w_L, w_R)$ defined previously. Thus, the one-dimensional Riemann solver is used twice in each space dimension.

Expressing (53) in terms of L_{1D}^G only leads to

$$L_{2D}^{G}(\Delta t) = I + (L_{x}^{G}(\Delta t) - I) \; L_{y}^{G}(\frac{\Delta t}{2})$$

$$+ (L_{y}^{G}(\Delta t) - I) \; L_{x}^{G}(\frac{\Delta t}{2}) \quad . \qquad (54.1)$$

Since $L_{1D}^{G}(\tau)$ is linear in τ, this may also be written as

$$L_{2D}^{G}(\Delta t) = I + (L_{x}^{G}(\Delta t) - I) \; \tfrac{1}{2}(L_{y}^{G}(\Delta t) + I)$$

$$(L_{y}^{G}(\Delta t) - I) \; \tfrac{1}{2}(L_{x}^{G}(\Delta t) + I) \; . \qquad (54.2)$$

Using the homogeneity property of the Euler equations and, therefore, of the Riemann solution, we may further work this out:

$$L_{2D}^{G}(\Delta t) = \tfrac{1}{2}[L_{x}^{G}(\Delta t) \; (L_{y}^{G}(\Delta t) + I) - L_{x}^{G}(\Delta t)$$

$$+ L_{y}^{G}(\Delta t) \; (L_{x}^{G}(\Delta t) + I) - L_{y}^{G}(\Delta t)] \; , \qquad (54.3)$$

This would reduce to Strang's splitting (52.1) if L_{1D}^{G} would have the distributive property. This, of course, is only true in the linear case.

3.3. Second-order schemes

The examples of the previous section teach us that it is possible to mimic two-dimensional wave-interactions by combinations of one-dimensional wave interactions. These schemes contain terms $\sim (\Delta t)^2$, but only have first-order accuracy. It is possible to apply the ideas of Section 3.1 and 3.2 to the second-order schemes of Section 2. This clearly involves more algebra and will not be carried out here. One of the reasons is that none of these two-dimensional schemes has yet been programmed. It remains to be shown in

practice if the more subtle ways of splitting like (53) are indeed preferable to a pure product operator like (52.2).

3.4. Related subjects

In two dimensions the grid plays an even more important role than in one dimension. Various ingredients of the schemes discussed in these lectures may be used more than once, in order to make decisions about refining the grid, moving the grid or just rotating the frame in which the solution of a one-dimensional Riemann problem is considered.

For the latter decision we may use the direction of the gradient of the solution - readily available from $\delta_x w$ and $\delta_y w$ in a second-order scheme - or the projection angle at which the initial values in a Riemann problem could be best connected ("best" in some least-squares sense) by a single running wave. The latter idea is due to Harten (private communication).

Moving a grid interface at the speed of the best-fitting single wave was realized in one dimension by Harten and Hyman (1982); two-dimensional results will soon follow. It appears that the improvement due to the grid movement is dramatic for a first-order scheme and not nearly so much for second-order schemes.

A two-dimensional extension of Roe´s matrix theory is being considered (Baines, M. J., (1982), University of Reading, United Kingdom, private communication).

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(a)

(b)
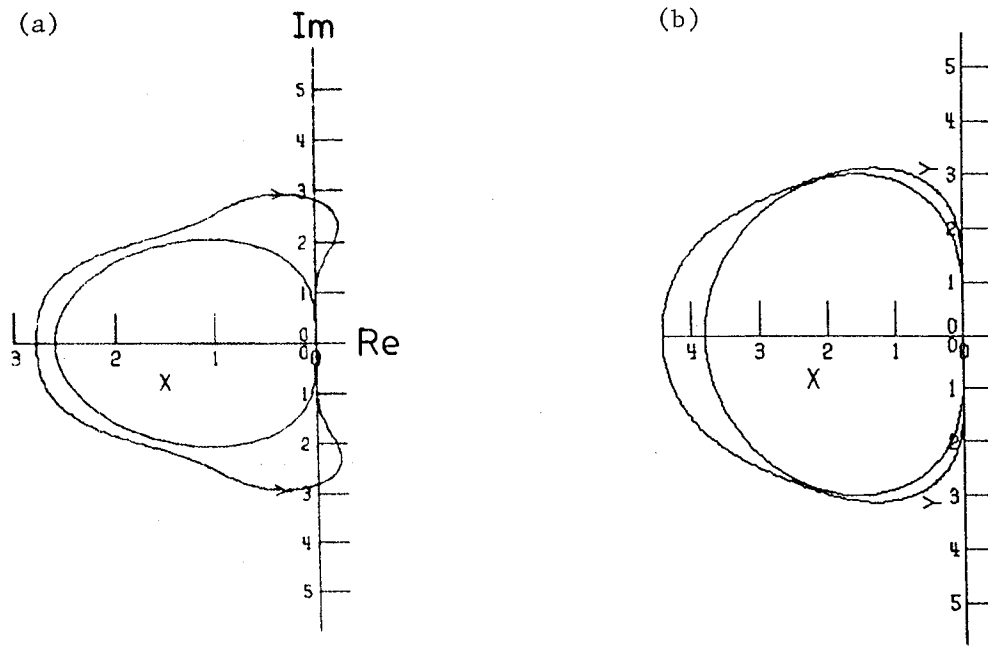
Fig. 1. Stability domain of four-step Runge-Kutta methods in the complex plane.

a) With $\alpha^{(1)} = \alpha^{(2)} = \alpha^{(3)} = \alpha^{(4)} = 1$. The inner contour is the locus of the Fourier transform of the second-order upwind spatial-differencing operator, for $\sigma = 1.3$.

b) With $\alpha^{(1)} = \alpha^{(2)} = 1$, $\alpha^{(3)} = .86$, $\alpha^{(4)} = .44$; $\sigma = 1.9$.
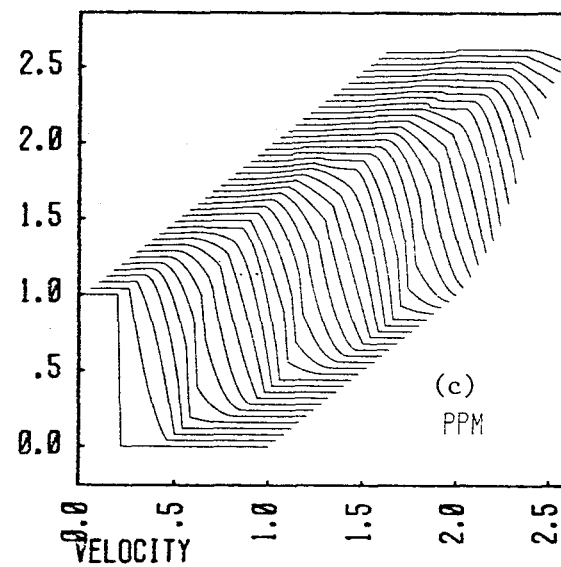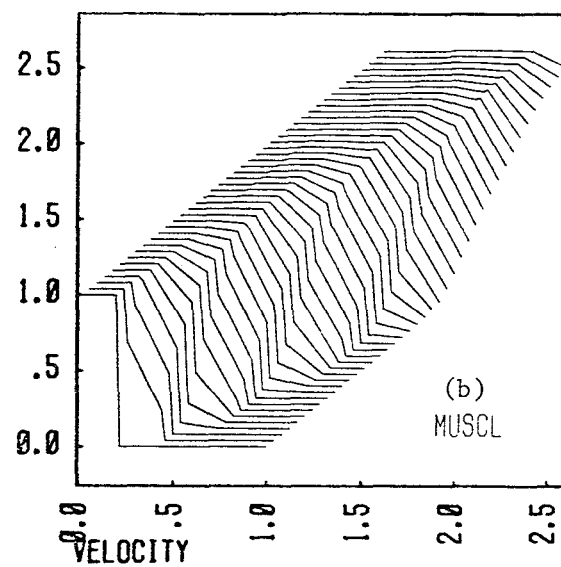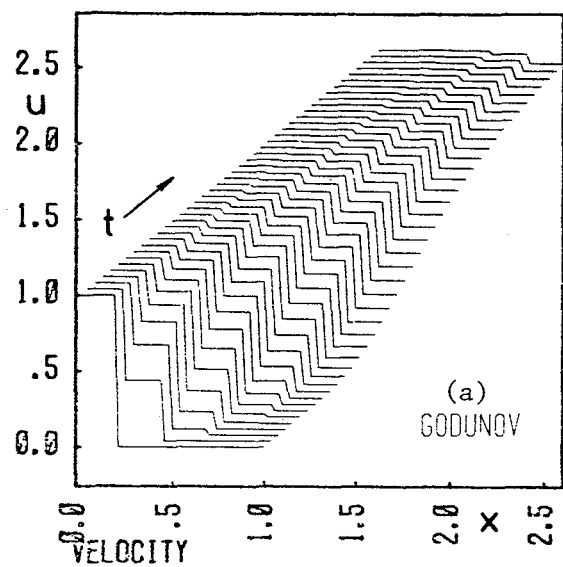
Fig. 2. Propagation of a one-dimensional shock, as represented by first-order (a), second-order (b) and third-order (c) upwind methods. Note that the overall distribution is always monotone. Reproduced from Woodward (1980).
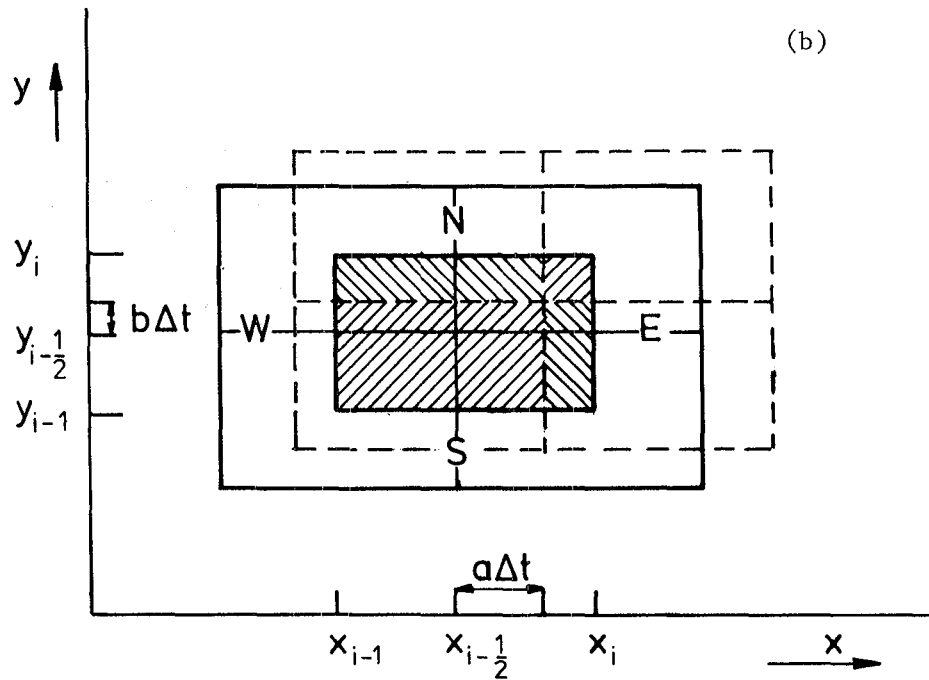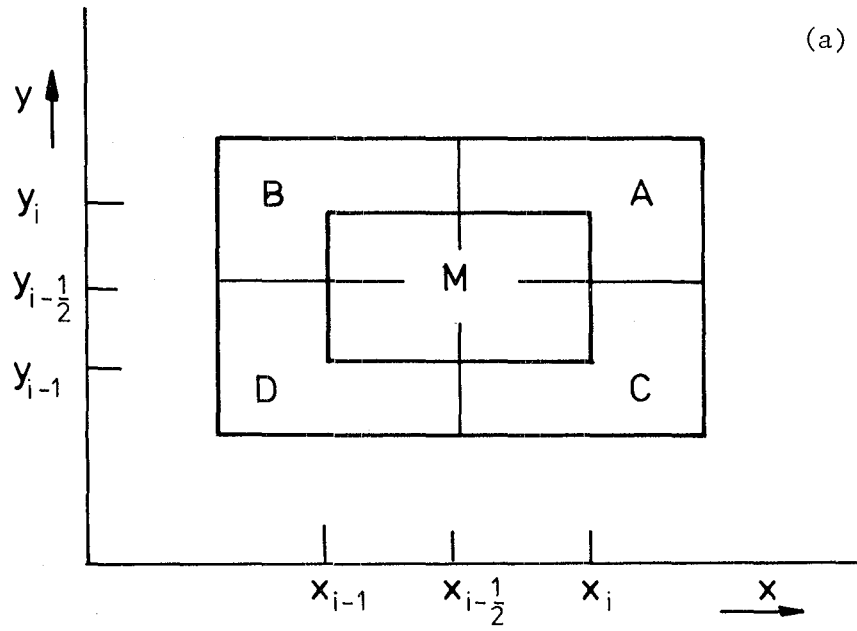
Fig. 3. Two-dimensional convection by the Lax-Friedrichs scheme. (a) Staggered grid of finite volumes. (b) Contours of the convected distribution after one time step (broken lines). The updated average value in zone M is an area-weighted average of the values in A, B, C and D; the areas are shaded distinctively.
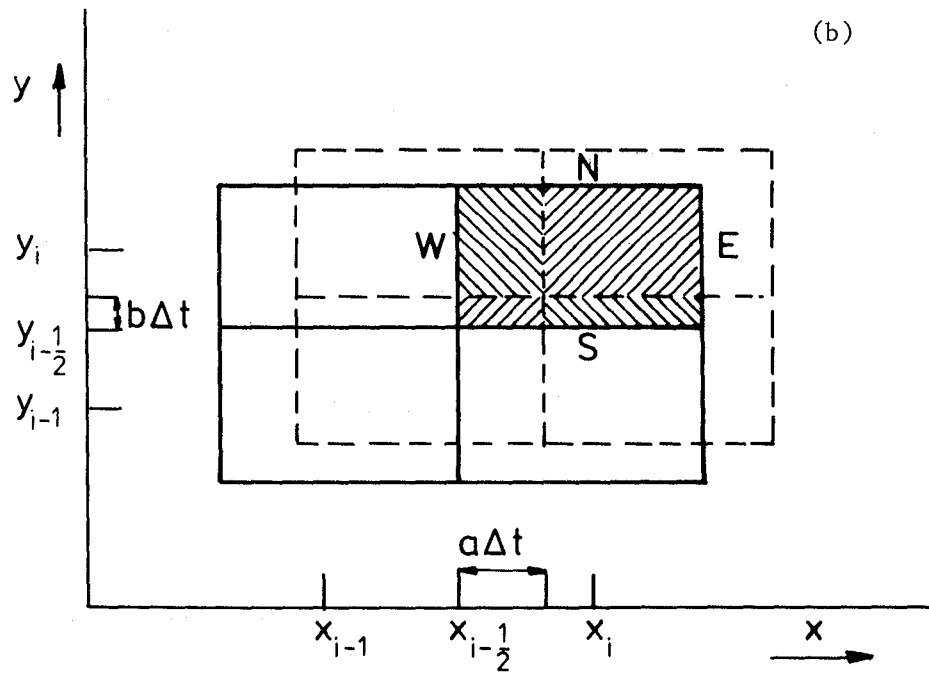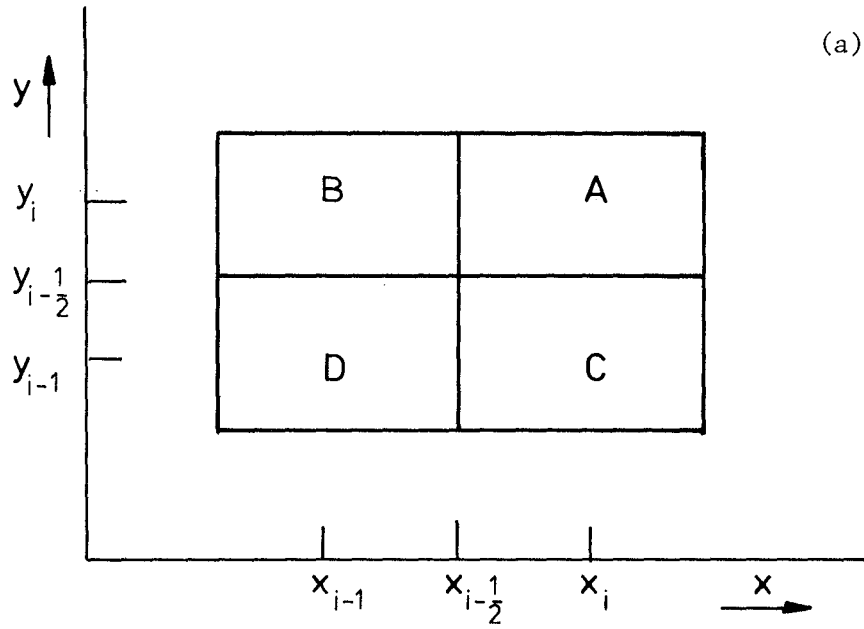
Fig. 4. Two-dimensional convection by Godunov's scheme. Same as Fig. 3, except updating is done in zone A.

16. Abstract

Lectures presented at the Von Karman Institute for Fluid Dynamics, Rhode-St-Genese, Belgium, in Lecture Series 1983-04 on Computational Fluid Dynamics.

1. Conservative dissipative difference schemes   p.1

2. The recognition and representation of discontinuities p.13

3. Multi-dimensional methods   p.18

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