Comparison of Different Numerical Methods for Calculating One-dimensional Unsteady Flows

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The following analysis compares the ability to depict the propagation of shocks, together with accuracy and computational cost of: several forms of the method of characteristics, the method of lines, explicit and implicit finite difference methods. In particular the propagation of a step- and a sine-function by the linear one-dimensional advection equation is considered. Thereby the frequently used method of Lax-Wendroff appears as a good compromise between simplicity, accuracy, speed, and robustness. Computing times reported by several authors dealing practical problems even confirm this statement. The method is simple in the sense that only three grid-points of the preceding time level are involved in the numerical solution belonging to a certain grid-point. It is robust since only moderate overshoot occurs in case of shocks or discontinuous initial conditions. Overshoot can be completely eliminated by the method of flux-correction due to Book, Boris and Hain.

1 Hyperbolic systems of conservation laws

Neglecting viscous forces, heat conduction and gravity one-dimensional unsteady flow in a tube of constant cross-section obeys the conservation of mass, momentum and energy. This leads to the following system of equations:

\[
\frac{\partial}{\partial t} \begin{pmatrix} Q \\ Qw \\ Q \left( e + \frac{w^2}{2} \right) \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} Qw \\ Qw^2 + p \\ Qw \left( e + \frac{w^2}{2} + \frac{p}{Q} \right) \end{pmatrix} = 0
\]

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(t = time coordinate, x = space coordinate, \( \rho \) = density, \( w \) = velocity, \( e \) = internal energy, \( p \) = pressure) which is of the form

\[
W_t + F_x = 0 \tag{1.2}
\]

with \( W \) and \( F \) a vector of dimension 3. The elements of \( W = W(x, t) \) are called the dependent variables, whereas \( x \) and \( t \) are called the independent variables. Since \( p = p(\rho, e) \) and \( \rho, w, e \) are expressible by the elements of \( W \), \( F \) is a function of \( W \)

\[
F = F(W) \tag{1.3}
\]

P. Lax and B. Wendroff (1960) call a system of the form (1.2) with (1.3) a system of conservation laws.

The system (1.2) is hyperbolic if all eigenvalues of the matrix

\[
F' = \frac{\partial F}{\partial W} \tag{1.4}
\]

are real. This turns out to be true for system (1.1). With (1.4) it can be written as a system of quasi-linear hyperbolic equations

\[
W_t + F' W_x = 0 \tag{1.5}
\]

The conservation law form of hyperbolic equations has the favourable property that conservative finite-difference methods applied to it produce solutions automatically satisfying the Rankine-Hugoniot relations across a shock, which greatly facilitates accurate shock calculation. We therefore assume the flow equations in this form.

In the following sections we consider numerical methods for determining approximate values of the solution \( W(x, t) \) of hyperbolic equations (1.2) with prescribed initial values \( W(x, 0) \) for \(-\infty < x < +\infty\).

2 The characteristic equations

If we follow a point moving from \( x \) to \( x + dx \) within the time interval \( dt \) the variation of the vector function \( W = W(x, t) \) is

\[
dW = W_t \, dt + W_x \, dx \tag{2.1}
\]

Using (1.5) to replace the time derivative by a space derivative we obtain

\[
dW = - \left( F' - \frac{dx}{dt} \right) W_x \, dt \tag{2.2}
\]

Let us now consider an arbitrary linear combination of the elements of \( dW \). We achieve this by scalar multiplication of (2.2) with some vector \( q \) of the same dimension as \( W \) (the superscript \( T \) denotes transposition)
Methods for Calculating One-dimensional Unsteady Flows

\[ q^T \, dW = - q^T \left( F' - \frac{dx}{dt} \right) W_x \, dt \]  

(2.3)

If \( \frac{dx}{dt} \) is an eigenvalue of \( F' \) and \( q^T \) a lefthand eigenvector of \( F' \), expression (2.3) gets very simple. We designate the \( \nu \)-th eigenvalue of \( F' \) with \( \gamma_\nu \) and the corresponding eigenvector with \( q_\nu \), that is

\[ q^T_\nu F' = q^T_\nu \gamma_\nu \]  

(2.4)

Note that in general \( \gamma_\nu \) and \( q_\nu \) depend on \( W \). If a solution \( W \) is known then

\[ \frac{dx}{dt} = \gamma_\nu (W) \]  

(2.5)

defines the \( \nu \)-th characteristic \( C_\nu \) and

\[ q^T_\nu (W) \frac{dW(x, t)}{dt} = 0 \]  

(2.6)

represents an ordinary differential equation along \( C_\nu \). Equations (2.5) and (2.6) for all characteristics together constitute the characteristic equations for system (1.2).

The vector \( q \) is not uniquely determined by (2.4). If it is possible to select it so that

\[ W(x, t) = 0 \text{ along } C_\nu \]  

(2.7)

then it follows from (2.6) that the expression

\[ q^T(W) \, W(x, t) \]  

(2.8)

is constant along the characteristic \( C_\nu \). It would have been intelligible to call (2.8) a Riemann invariant in this case. In fact this denotation is used only if \( C_\nu \) represents a path of sound waves.

Numerical solutions of the characteristic equations may be attempted on a grid of characteristics or on a rectangular coordinate grid.

3 Solution of the characteristic equations on a grid of characteristics

Let us consider the case of two dependent variables. Then there are two characteristics through one point. Suppose the solution is known at points \( P_1 \) and \( P_2 \) not located on the same characteristic (see Fig. 1). Let \( P \) be the point of intersection of characteristic \( C_1 \) through \( P_1 \) and \( C_2 \) through \( P_2 \). Then the characteristic equations (2.5) and (2.6) can be approximated to first order, which leads to the linear system of equations

\[
\begin{align*}
x(P) - x(P_v) &= \gamma_v(P_v)(t(P) - t(P_v)) \\
q^T_v(P_v)(W(P) - W(P_v)) &= 0
\end{align*}
\]

(3.1)

\( v = 1,2 \)
with the unknowns W(P), x(P), t(P). By repeated application of this procedure starting from a line I in (x, t) space along which values for W are given, the solution is obtained on the nodes of a grid of characteristics. This is the method of Massau (G. E. Forsythe and W. R. Wasow, 1960, pp. 64–65).

Fig. 1: Grid of characteristics for calculating the solution at point X. AB is the domain of dependence on line I. P is the point of intersection of characteristic C₁ through P₁ and C₂ through P₂.

Bild 1: Gitter aus Charakteristiken für die Berechnung der Lösung am Punkt X. AB ist das Abhängigkeitsgebiet auf Linie I. P ist der Schnittpunkt von Charakteristik C₁ durch P₁ und C₂ durch P₂.

Note that the exact solution at a point X depends only on values of W on line I within the smallest interval AB on I containing the intersections of all characteristic lines through this point X. AB is called the domain of dependence on I of the exact solution at X.

A second order method can be obtained replacing \( \gamma \) and \( q \) by averages over \( P \) and \( P \). The resulting nonlinear equations may be solved by iteration. Such a procedure has been described by Hartree (M. Lister, 1960) and used by N. E. Hoskin and B. D. Lambourn (1971) for non-isentropic one-dimensional unsteady flow.

R. A. Ansorge (1963) has constructed higher order methods in analogy with the Adam’s methods for ordinary differential equations. Because the number of points to be considered grows exponentially with the distance from the line of given initial data, it is practicable not far from this line only.

Higher order is more easily achieved by extrapolation. This is done in the algorithms of R. R. Smith and D. McCall (1970) and W. Busch et al. (1975). Smith-McCall use Massau’s method with extrapolation to the limit from re-
sults of two interval halvings leading to a method of order three. Busch et al. proceed from "the midpoint rule started by Euler's method", which is related to Hartree's second order method. Since extrapolation works satisfactorily only if the exact solution is sufficiently differentiable, the numerical solution becomes rather erroneous in the presence of shocks.

Solving the characteristic equations on a grid of characteristics is generally referred to as the method of characteristics. Its advantages are:

- Discontinuous initial data and shock waves do not lead to solutions with overshoot. Details are not smeared.
- Large steps are possible since the step length is not restricted by a stability criterion.
- The method of characteristics is exact in the constant coefficient case with two dependent variables, regardless of eventual discontinuities in the initial data.

Disadvantages are:

- Special procedures for shock calculations are necessary.
- Not only the solution at node points but also the node points themselves must be determined. Interpolation is required if the solution is asked for on a coordinate grid.
- For more than two dependent variables the points $P_v$ in (3.1) are not as free as for two dependent variables and the complexity of the computation increases greatly.

4 Solution of the characteristic equations on a coordinate grid

From now on we examine methods which directly yield approximate values $W_j^n$ of the solution $W(x, t)$ at the nodes $(j\Delta x, n\Delta t)$ of an axially parallel rectangular net.

In order to calculate approximate values $W_{j}^{n+1}$ at the line $t = (n+1)\Delta t$ from values at the nodes of the preceding line $t = n\Delta t$, we place the points $P$ and $P_v$ as indicated in Fig. 2 and use equations (3.1) with $\gamma_v$ and $q_v$ evaluated at $P_0$, not at $P_v$. Now $x(P)$, $t(P)$ and $t(P_v)$ are known, $W(P)$ and $x(P_v)$ are unknown, $W(P_v)$ is estimated from $W(P_+), W(P_0), W(P_-)$ by linear interpolation. This method is of first order and has been described by R. Courant, E. Isaacson and M. Rees (1952). R.S. Benson et al. (1964) calculated one-dimensional flows with a slightly modified version of it. An other modified form with $\gamma_v$ and $q_v$ replaced by averages over $P$ and $P_v$ has been given by D.R. Hartree (1958) and used by R.I. Issa and D.B. Spalding (1972) for one-dimensional flow calculations. A second order method is obtained if in addition quadratic instead of linear interpolation is used (D.R. Hartree, M. Lister, 1960). In the constant coefficient case this is identical to the method of Lax-Wendroff.
Fig. 2: Coordinate grid for calculating the solution at node point P of line \( t = (n+1)\Delta t \). The characteristics \( C_1 \) and \( C_2 \) intersect the line \( t = n\Delta t \) (with node points \( P_- \), \( P_0 \), \( P_+ \)) at the points \( P_1 \) and \( P_2 \) respectively.

Bild 2: Koordinatengitter für die Berechnung der Lösung an Knotenpunkt P der Linie \( t = (n+1)\Delta t \). Die Charakteristiken \( C_1 \) und \( C_2 \) schneiden die Linie \( t = n\Delta t \) (mit Knotenpunkten \( P_- \), \( P_0 \), \( P_+ \)) an den Punkten \( P_1 \) bzw. \( P_2 \).

Obviously the methods just mentioned relate the solution at the point P to values on section \( P_- P_+ \) of the line \( t = n\Delta t \) (Fig. 2), that is \( P_- P_+ \) is the domain of dependence on \( t = n\Delta t \) of the numerical solution at P. The respective domain of dependence of the exact solution is the smallest interval on the line \( t = n\Delta t \) containing all points \( P_v \). Since a necessary condition of stability due to Courant-Friedrichs-Lewy is that the domain of dependence of the numerical solution covers up the domain of dependence of the exact solution, we get here the following necessary stability criterion

\[
x(P_-) \leq x(P_v) \leq x(P_+) \tag{4.1}
\]

which must be satisfied for all \( v \).

Let us henceforth illustrate numerical methods by writing respective formulas for the linear one-dimensional scalar advection equation, that is for scalar \( W \) and \( F', F' \) being constant. Then \( W \) is a Riemann invariant type quantity and \( F' \) is the characteristic speed.

Leaving points P and \( P_1 \) as in Fig. 2, equation (3.1) for \( v = 1 \) now reads

\[
\begin{align*}
{j}\Delta x - x(P_1) &= F'\Delta t \\
W^{n+1}_v - W(P_1) &= 0
\end{align*}
\tag{4.2}
\]

We introduce the so-called Courant number

\[
\alpha = \frac{F'\Delta t}{\Delta x} \tag{4.3}
\]

which is the path length in units of \( \Delta x \) a perturbation of \( W \) propagates within time \( \Delta t \). With this we get from (4.2)
and
\[ x(P_j) = (j - \alpha) \Delta x \] \hspace{1cm} (4.4)
\[ W_j^{n+1} = W_{j-\alpha}^n \] \hspace{1cm} (4.5)
defining that \( W_{j-\alpha} \) is an approximation for \( W((j-\alpha)\Delta x, n\Delta t) \) for nonintegral values \( j-\alpha \) too. Equation (4.5) merely expresses the fact, that in the case considered here \( W \) remains constant along the characteristic.

Approximation of \( W_{j-\alpha} \) by linear interpolation along the line \( t = n\Delta t \) yields the first order method
\[ W_j^{n+1} = W_j^n - (\alpha - [\alpha]) (W_{j-[\alpha]}^n - W_{j-[\alpha]^{-1}}^n) \] \hspace{1cm} (4.6)
which K.V. Roberts and N.O. Weiss (1966, p. 275) attribute to Lelevier. Here \([\alpha]\) is the largest integer not exceeding \( \alpha \). For \( |\alpha| \leq 1 \) this becomes the method of R. Courant, E. Isaacson and M. Rees (1952, P.J. Roache, 1972, p. 64):
\[ W_j^{n+1} = W_j^n - \alpha \times \begin{cases} (W_j^n - W_{j-1}^n), & \alpha \geq 0 \\ (W_{j+1}^n - W_j^n), & \alpha < 0 \end{cases} \] \hspace{1cm} (4.7)
Approximation of \( W_{j-\alpha} \) by symmetric quadratic interpolation along the line \( t = n\Delta t \), that is by averaging the quadratic interpolants of the three values (see Fig. 3)
\[ W_j = W_{j-[\alpha]-2}, W_{j-[\alpha]-1}, W_{j-[\alpha]} \]
and
\[ W_{j-[\alpha]-1}, W_{j-[\alpha]}, W_{j-[\alpha]+1} \]
respectively at the point \( x = (j - \alpha) \Delta x \), yields the second order method
\[ W_j^{n+1} = W_j^n - \frac{\alpha - [\alpha]}{4} (W_{j-[\alpha]+1}^n + 3 W_{j-[\alpha]}^n - 5 W_{j-[\alpha]-1}^n + W_{j-[\alpha]-2}^n) \]
\[ + \frac{(\alpha - [\alpha])^2}{4} (W_{j-[\alpha]+1}^n - W_{j-[\alpha]}^n - W_{j+[\alpha]-1}^n + W_{j+[\alpha]-2}^n) \] \hspace{1cm} (4.9)
It produces solutions with phase error zero in the average over \( \alpha \). For \( |\alpha| \leq 1 \) it becomes the zero average phase error method of J.E. Fromm (1968, P.J. Roache, 1972, p. 104).

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**Fig. 3:** Determination of the Riemann invariant type quantity at node point \( j \) of line \( t = (n+1)\Delta t \) by going back on the characteristic \( C_1 \) and symmetric interpolation along the line \( t = n\Delta t \).

**Bild 3:** Bestimmung der Riemann-Invarianten am Knotenpunkt \( j \) der Linie \( t = (n+1)\Delta t \) durch Zurückgehen entlang der Charakteristik \( C_1 \) und symmetrischer Interpolation entlang der Linie \( t = n\Delta t \).
Analogously cubic interpolation leads to the third order method

\[
W_{j}^{n+1} = W_{j}^{n} - \frac{[a] - \alpha}{6} \left( 2 W_{j-[a]+1}^{n} + 3 W_{j-[a]}^{n} - 6 W_{j-[a]-1}^{n} + W_{j-[a]-2}^{n} \right)
\]

\[
+ \frac{(\alpha - [a])^2}{6} \left( 3 W_{j-[a]+1}^{n} - 6 W_{j-[a]}^{n} + 3 W_{j-[a]-1}^{n} \right)
\]

\[
- \frac{(\alpha - [a])^3}{6} \left( W_{j-[a]+1}^{n} - 3 W_{j-[a]}^{n} + 3 W_{j-[a]-1}^{n} - W_{j-[a]-2}^{n} \right)
\]

which for \(| \alpha | \leq 1\) is the "QUICKEST" method of B. P. Leonard (1979) with equidistant grid spacing.

In principle the grid spacing need not be equidistant (see e.g. B. P. Leonard, 1979) and any appropriate interpolation method could be used.

According to P. Wesseling (1973) the method of Courant-Isaacson-Rees and the method of Fromm in some sense optimally depict the propagation of a discontinuity in the form of a step function. In fact overshoot resulting from discontinuities does not occur with the methods of Courant-Isaacson-Rees and Lelevier, it is small with Fromm's and Leonard's method, whereas with Hartree's second order method it is as large as with the method of Lax-Wendroff.

There is no commonly accepted name for the type of methods discussed in this section. Candidates are proposedly the designations "methods of characteristics with fixed time intervals" following M. Lister (1960), "mesh-methods of characteristics" following R. S. Benson et al. (1964), or "hybrid methods" following R. I. Issa and D. B. Spalding (1972). Other authors call them "characteristic interpolation type schemes" (P. Wesseling, 1973), "kinds of the method of characteristics" (W. Hackbusch, 1977), and "modified methods of characteristics" (H. Ehlich, F. Kruse and W. Stark, 1978).

Advantages of these methods are:
- No attention need be paid to the position of shocks. In general they cause only small overshoot.
- The methods are easily generalized to more than two dependent variables.
- Large time steps are possible if interpolation is done on a whole line in space.

Disadvantages are:
- The calculation is easy with Riemann type variables. If it is to be performed in terms of an arbitrary set of dependent variables, eigenvalues and eigenvectors of \( F' \) are needed at each node.

The order of accuracy may again be raised by extrapolation to the limit (see M. Lister, 1960, pp. 173–174 and W. Hackbusch, 1977).

Solution methods of the characteristic equations on a coordinate grid are indispensable for a correct treatment of boundary conditions in conjunction with finite difference methods (see A. M. Burns, 1978 and M. Goldberg and E. Tadmor, 1978).
5 The method of lines

Discretizing the spatial variable and replacing spatial derivatives by difference quotients our system of partial differential equations (1.2) transforms into a system of ordinary differential equations, which can be solved by any suitable numerical method. This is called the method of lines. Due to G. E. Forsythe and W. R. Wasow (1960, p. 178) this method has been used a good deal in the Soviet Union. Searching for universal algorithms for the numerical solution of partial differential equations it has recently attracted attention also in the United States and presently there is general purpose software available (R. F. Sincovec and N. K. Madsen, 1975). An application to the calculation of one-dimensional unsteady flow can be found in a paper of M. Ryti (1976).

With the method of lines special care must be taken of the formulation of boundary conditions. Since for the numerical solution of the generated system of ordinary differential equations the time variable in fact is discretized too, we finally obtain full finite difference methods. Many of the known finite difference methods can be thought of as generated in this way. Let us illustrate this on the basis of equations (1.2).

Considering the approximate solution at points \( x = j \Delta x \) as functions \( W_i(t) \) of time and using central differences (1.2) becomes the system of ordinary differential equations

\[
\frac{dW_i}{dt} = - \frac{F(W_{i+1}) - F(W_{i-1})}{2 \Delta x}
\]  

(5.1)

For constant \( F' \) the Jacobi Matrix of the right hand side of (5.1) is

\[
- \frac{F'}{2 \Delta x}
\]

(5.2)

Since it is skew-symmetric all eigenvalues are purely imaginary. Assuming scalar \( F' \) one can show (see e.g. R. Zurmühl, 1961, p. 224) that they are all located between the two limiting points \( \pm iF'/\Delta x \) in the complex plane. Thus the solution of (5.1) is representable as a linear combination of pure oscillations

\[ e^{i\lambda t} \]

(5.3)
with angular frequencies $\omega$ satisfying
\[ -\left| \frac{F'}{\Delta x} \right| \leq \omega \leq +\left| \frac{F'}{\Delta x} \right| \] (5.4)
and only those integration methods come into question here, which remain stable for pure oscillations. Optimal methods in this sense have been devised by P.J. van der Houwen (1972).

The following table gives an overview of the most important methods for the numerical integration of ordinary differential equations:

<table>
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<tr>
<td>Implicit Runge-Kutta methods</td>
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The first-order member of the family of explicit Runge-Kutta methods is the forward Euler method (L. Lapidus and J.H. Seinfeld, 1971, p. 47), which applied to (5.1) produce the finite difference method
\[ W_j^{n+1} = W_j^n - \frac{\Delta t}{2\Delta x} (F_j^{n+1} - F_j^{n-1}) \] (5.5)
It is unconditionally unstable because the forward Euler method is not stable for pure oscillating solutions. It can be made stable for $|\alpha| \leq 1$ by adding a damping term. In this way it becomes the method of Lax, the first-order member of a family of prominent finite difference methods, which are analogs of explicit Runge-Kutta methods.

A representative of explicit multistep methods is the midpoint rule (L. Lapidus and J.H. Seinfeld, 1971, p. 15). It is second-order accurate and stable only for pure oscillations of the type (5.3) under the condition that
\[ |\omega \Delta t| \leq 1 \] (5.6)
Applying it to (5.1) directly leads to the well-known leapfrog method, stable for $|\alpha| \leq 1$. This follows from (5.4) and (5.6).
Use of the implicit trapezoidal rule, stable for pure oscillations of arbitrary
frequency, yields the method of Crank-Nicholson, a typical example for an
implicit finite difference method with unconditional stability.

Advantages of the method of lines are its universal applicability and the
prospective profit from using highly developed software for ordinary differen-
tial equations. Its disadvantage is the difficulty for proper treatment of boun-
dary conditions.

6 Explicite finite difference methods

In this section we shall consider methods which allow the explicit calculation
of approximate values \( W_j^{n+1} \) of the solution at certain node points \((j\Delta x, (n+1)\Delta t)\) of a rectangular grid from known exact or approximate values \( W_j^n \)
of the solution at other node points \((j'\Delta x, n'\Delta t)\) preferably belonging to the
past \((n' < n+1)\). No eigenvectors need be calculated. Eigenvalues are re-
quired only for testing stability conditions. Here explicit means that no linear
or nonlinear equations are solved.

One of the most important finite difference methods is the method of
P. Lax and B. Wendroff (1960), which we write in the form

\[
W_j^{n+1} = W_j^n - \frac{1}{2} \left( \frac{\Delta t}{\Delta x} \right) (F_{j+1}^n - F_{j-1}^n)
+ \frac{1}{4} \left( \frac{\Delta t}{\Delta x} \right)^2 \left\{ (F_{j+1}^n + F_{j-1}^n) (F_{j+1}^n - F_{j-1}^n) - (F_{j+1}^n + F_{j-1}^n) (F_{j+1}^n - F_{j-1}^n) \right\}
\]

in accordance with J. Gary (1964, p. 9, see also G. Zehnder, 1971, and
P.J. Roache, 1972, p. 248). It is second-order accurate and stable for \( |\alpha| \leq 1 \).

The one-step form (6.1) is advantageous only if the evaluation of \( F_j^n = F'(W_j^n) \) in addition to \( F_j^n = F(W_j^n) \) does not bring about much additional com-
puting cost.

There are numerous two-step versions of this method which do not require
evaluation of \( F' \). A. Lerat and R. Peyret (1973) have united them into a two-
parametric family of second-order methods identical to the one-step form
(6.1) in case of constant \( F' \). They can be considered members of a more gen-
eral family of methods with the following properties:

- They are of equal order in space and time, even in the nonlinear case.
- They are explicit two-level methods (for the designation «two-level» see
e.g. P.J. Roache, 1972, p. 75). The solution at time level \( t = (n+1)\Delta t \) is en-
tirely calculated from the solution at time level \( t = n\Delta t \).
- They consist of several stages called steps. In each stage the function \( F(W) \)
is evaluated once per node point.
This family of explicit, multistep, two-level finite difference methods (related to the family of explicit multistage Runge-Kutta methods for ordinary differential equations) contains the following members:


  \[ W_{j+1}^{n+1} = W_j^n - \frac{\Delta t}{2\Delta x} (F_{j+1}^n - F_{j-1}^n) + \frac{\alpha}{4} (W_{j+1}^n - 2W_j^n + W_{j-1}^n) \]  

  (6.2)

  It is stable if \(|\alpha| \leq \sqrt{\omega/2}\) and \(0 \leq \omega \leq 2\).


  \[ W_{j+1}^{n+1} = \frac{1}{2} (W_{j+1}^n + W_j^n) - \frac{\Delta t}{2\Delta x} (F_{j+1}^n - F_j^n) \]  

  \[ W_j^{n+1} = W_j^n - \frac{\Delta t}{\Delta x} (F_{j+1}^n - F_{j-1}^n) \]  

  (6.3)

  It is stable for \(|\alpha| \leq 1\). In fact the whole two-parametric family of Lerat-Peyret could be inserted here, including the noncentered method of McCormack (P.J. Roache, 1972, p. 253) and the centered method of A. Lerat and R. Peyret (1973).

- **The method of V. V. Rusanov** (1970), S.Z. Burstein and A.A. Mirin (1970) (three-step, third order; we arbitrarily define the free parameter \(\tau_1 = \frac{1}{3}\), see S.Z. Burstein and A.A. Mirin, 1970, p. 552):

  \[ W_{j+1}^{n+1} = \frac{1}{2} (W_{j+1}^n + W_j^n) - \frac{\Delta t}{3\Delta x} (F_{j+1}^n - F_j^n) \]  

  \[ W_j^{n+1} = W_j^n - \frac{\Delta t}{3\Delta x} (F_{j+1}^n - F_{j-1}^n) \]  

  (6.4)

  \[ W_{j+1}^{n+1} = W_j^n - \frac{\Delta t}{24\Delta x} \left\{ 9(F_{j+1}^n - F_{j-1}^n) + 7(F_{j+1}^n - F_j^n) - 2(F_{j+2}^n - F_{j-2}^n) \right\} \]  

  \[- \frac{\alpha}{16} \left( W_{j+2}^n - 4W_{j+1}^n + 6W_j^n - 4W_{j-1}^n + W_{j-2}^n \right) \]

  It is stable if \(|\alpha| \leq 1\) and \(2 \alpha^2(4-\alpha^2)/3 \leq \omega \leq 2\). In the constant coefficient case it is identical to the noncentered third-order method of R.F. Warming, P. Kutler and H. Lomax (1973, pp. 191–192).

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\[ W_{j+1}^{n+1} = \frac{1}{2} (W_j^{n+1} + W_j^n) - \frac{\Delta t}{2\Delta x} (F_{j+1}^n - F_j^n) \]

\[ W_j^{n+2} = \frac{1}{8} \left\{ 10 W_j^n - (W_{j+1}^n + W_{j-1}^n) \right\} - \frac{\Delta t}{2\Delta x} (F_{j+1}^{(3)} - F_{j}^{(1)}) \]

\[ W_{j+2}^{(3)} = \frac{1}{16} \left\{ 9 (W_{j+1}^n + W_j^n) - (W_{j+2}^n + W_{j-1}^n) \right\} \]

\[ - \frac{\Delta t}{8\Delta x} \left\{ 8 (F_{j+1}^{(2)} - F_j^{(2)}) + 3 (F_{j+1}^n - F_j^n) - (F_{j+2}^n - F_j^n) \right\} \]

\[ W_j^{n+1} = W_j^n - \frac{\Delta t}{96\Delta x} \left\{ 16 (F_{j+1}^{(3)} - F_j^{(3)}) + 16 (F_{j+1}^{(2)} - F_j^{(2)}) \right\} \]

\[ + 56 (F_{j+1}^{(1)} - F_j^{(1)}) - 8 (F_{j+1}^{(2)} - F_j^{(2)}) + 10 (F_{j+1}^n - F_j^n) - (F_{j+2}^n - F_j^n) \right\} \]

This method is stable for \(|\alpha| \leq 1\) (S. Abarbanel et al., 1975, p. 338).

Explicit multistep two-level methods of arbitrary order have been presented by S. Abarbanel and D. Gottlieb (1973).

The most important finite difference method involving more than two time levels within one time step is the leapfrog method (P. J. Roache, 1972, p. 54).

\[ W_j^{n+1} = W_j^n - \frac{\Delta t}{\Delta x} (F_{j+1}^n - F_j^n) \]  

(6.6)

It is second-order accurate and stable for \(|\alpha| \leq 1\). It requires only one evaluation of \(F(W)\) per node point and shows no amplitude error. Unfortunately the method becomes unconditionally unstable as soon as the hyperbolic equations (1.2) contain the least perturbation e.g. a friction or a viscosity term on the right-hand side. Stability can be regained by a proposal of E.C. Du-Fort and S.P. Frankel (1953, p. 148, P.J. Roache, 1972, p. 61). That is

replace \(W_j^n\) by \(\frac{1}{2} (W_j^{n+1} + W_j^{n-1})\)  

(6.7)

in the difference approximation of the perturbation term. In the most of the practical important cases the resulting implicit equation for \(W_j^{n+1}\) is easy to solve.

Without reducing accuracy the leapfrog method can be applied to half of the node points only constituting a staggered mesh. The method is not self-starting. For the first step in time a two-level method is needed. A method of equivalent quality which does not have this drawback is the hopscotch method of A.R. Gourlay and J.L. Morris (1972) derived from the method of Lax in the form (6.2). It is stable for \(|\alpha| \leq 1\) and \(\omega \geq 0\). The method requires only one evaluation of \(F(W)\) for every second node point and is second order accurate for \(\omega = 0\).

Explicit three-level methods of higher order in space similar to leapfrog have been investigated by K.V. Roberts and N.O. Weiss (1966) and
H.O. Kreiss and J. Oliger (1972). There are two- and three-level methods which are related to the predictor-corrector methods of ordinary differential equations. They are suitably called iterative methods (J. Gary, 1964, p. 15, S. Abarbanel and G. Zwas, 1969) although practically only one iteration is carried out.

So far we have considered finite difference methods symmetric in space. If all eigenvalues of $F'$ have equal sign, then so-called upwind difference schemes are feasible. Such methods may be derived from those described in section 4 replacing $\alpha vW$ by $(\Delta t/\Delta x)v(F')^{-1}F$. They are meaningful for flow calculations in the supersonic region. A two-step second-order upwind difference method which does not require evaluation of $F'$ has been devised by R.F. Warming and R.M. Beam (1976).

The finite difference methods (6.1) until (6.6) are conservative in the sense that the sum over all node values of $W$ at time level $(n+1)$ differs from the sum over all node values of $W$ at previous time steps by a small number of boundary terms only. As already noted in section 1 this property is helpful for accurate shock calculation. Advantages of explicite finite difference methods are:

- No care must be taken of the location of shocks.
- No eigenvectors have to be computed. Eigenvalues are needed solely for testing stability conditions.
- No linear or nonlinear equations are to be solved.

Disadvantages are:

- In the presence of shocks the methods of higher than first order produce considerable overshoot.
- Time steps are restricted by a stability criterion.

Methods (6.1) until (6.6) are unstable for $|\alpha| > 1$ that is for $\Delta t > \Delta x/|\gamma_{\text{max}}|$ in the nonscalar case ($\gamma_{\text{max}} =$ eigenvalue of $F'$ with maximal absolute value). Methods (6.1), (6.3), (6.5) are stable for $|\alpha| \leq 1$, methods (6.2) and (6.4) can be made stable for $|\alpha| \leq 1$ by choosing $\omega = 2$.

7 Implicit finite difference methods

The restriction on time steps can be overcome by admitting the solution of implicit linear or nonlinear equations in the process of calculating approximate values $W^{n+1}_j$ at time level $n+1$ from values $W^n_j$ at previous time levels $n' < n+1$.

The following two methods of this type originate in applying the method of lines with the backward Euler and the trapezoidal rule as integrator:

- The fully implicit method (P.J. Roach, 1972, p. 84)
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\[ W_{j}^{n+1} = W_{j}^{n} - \frac{\Delta t}{2\Delta x} (F_{j+1}^{n+1} - F_{j-1}^{n+1}) \]  
(7.1)

used for the analysis of flood propagation in channel systems by V. Desikan (1966) and


\[ W_{j}^{n+1} = W_{j}^{n} - \frac{\Delta t}{4\Delta x} \left\{ (F_{j+1}^{n} - F_{j-1}^{n}) + (F_{j+1}^{n+1} - F_{j-1}^{n+1}) \right\} \]  
(7.2)


For one-dimensional unsteady flow calculations D. V. von Rosenberg, D. L. Beauchamp and J. W. Watts (1968) and J. D. Ledger (1975) used the centered difference method

\[ \frac{1}{2} \left\{ \frac{W_{j+1}^{n+1} - W_{j+1}^{n}}{\Delta t} + \frac{W_{j}^{n+1} - W_{j}^{n}}{\Delta t} \right\} + \frac{1}{2} \left\{ \frac{F_{j+1}^{n+1} - F_{j}^{n+1}}{\Delta x} + \frac{F_{j+1}^{n} - F_{j}^{n}}{\Delta x} \right\} = 0 \]  
(7.3)


Implicit methods are appropriate if the time step is more restricted by stability criterions of explicit methods than by accuracy requirements. Since accuracy is determined by derivatives of the solution, the application of implicit methods is likely to be successful in cases where the solution varies slowly in space and time or where the important effects propagate slowly with respect to the acoustic waves. This occurs seldom with unsteady flows, where the system changes significantly in a time \( \Delta t = \Delta x / |\gamma_{\text{max}}| \), so that there is no reason for larger time steps (see R. D. Richtmyer and K. W. Morton, 1967, p. 295).

Thus the excessive good performance of an implicit method on unsteady flow problems reported by D. V. von Rosenberg et al. (1968) seems to result from poor programming of the method compared with, a suspicion confirmed by later work (J. D. Ledger, 1975).

8 Controlling overshoot

Numerical evidence shows that in the presence of discontinuous initial values or shock waves finite difference methods of higher than first order produce solutions with non-physical overshoot. There are many proposals to reduce it:

- Add physical viscosity terms with modified and strongly amplified viscosity, acting on momentum and energy components only (for a short review see P.J. Roache, 1972, pp. 232-235 and p. 254).

- Add damping terms which uniformly act on all components of \( W \).
Addition of a second order damping term e.g. changes the solution $W_{j}^{n+1}$ to the damped solution

$$\bar{W}_{j}^{n+1} = W_{j}^{n+1} + \frac{\omega}{4} (W_{j+1}^{n} - 2W_{j}^{n} + W_{j-1}^{n})$$

(8.1)

with $\omega$ some positive constant of the order of magnitude 1. This introduces an error of second order. Similarly the nonlinear damping proposed by P. Lax and B. Wendroff (1960) acts in the neighbourhood of a discontinuity (R. D. Richtmyer and K. W. Morton, 1967, pp. 335–336). It introduces an error merely of order three, but is inactive with constant $F'$. Damping terms change the stability properties of a method sometimes for the better, as with (6.2) and (6.4), frequently to the worse.


Smoothing reduces amplitudes only, not altering phases and not deteriorating stability. Fourth order smoothing e.g. changes the solution $W_{j}^{n+1}$ to

$$\bar{W}_{j}^{n+1} = W_{j}^{n+1} - \frac{\omega}{16} (W_{j+2}^{n} - 4W_{j+1}^{n} + 6W_{j}^{n+1} - 4W_{j-1}^{n+1} + W_{j-2}^{n+1})$$

(8.2)

introducing an error of fourth order ($0 \leq \omega \leq 2$).

- In the neighbourhood of the discontinuity switch to a first order method (A. Harten and G. Zwas, 1972).

Out of a two-parametric family of methods the method of Lerat-Peyret shows optimal damping and practically no overshoot for shock solutions of the Burger equation. Nevertheless in case of constant $F'$ the method is identical to the method of Lax-Wendroff and produces the same amount of overshoot.


With this method in a first stage the solution is damped strongly enough. Then in a second stage damping is revoked but, with the aid of a nonlinear correction, only as far as no overshoot occurs.


9 Comparison of methods

Let us now compare methods by means of the following two problems:

(A) Propagation of a step function by the linear one-dimensional scalar advection equation, that is (1.2) with $F' = \text{const}$ and the initial condition
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\[
W(x, 0) = \begin{cases} 
1, & -\infty < x \leq 0 \\
0, & 0 < x < +\infty
\end{cases}
\] (9.1)

With this problem we examine the development of overshoot of numerical solutions over ten time steps with different Courant-numbers, that is with \(\alpha = 0.1, 0.3, 0.5, 0.7, 0.9\) for explicit methods and \(\alpha = 0.1, 0.5, 0.9, 1.3, 1.7\) for implicit methods.

(B) Propagation of a Fourier-component with wave-number \(k = \frac{2\pi}{\lambda}\) (\(\lambda = \text{wavelength}\)) by the linear one-dimensional scalar advection equation, that is (1.2) with \(F' = \text{const}\) and the initial condition

\[
W(x, 0) = e^{ikx}, \quad -\infty < x < +\infty
\] (9.2)

Advancing the true solution of this problem one time step is equivalent to multiplying it by the amplification factor

\[
G(\alpha, \theta) = e^{-i\alpha \theta}
\] (9.3)

with \(\theta = k\Delta x\), whereas application of the method of Lax (6.2) as an example corresponds to multiplying it by

\[
G_{\text{Lax}}(\alpha, \theta) = 1 - i\alpha \sin \theta - \frac{\omega}{2} (1 - \cos \theta)
\] (9.4)

If in accordance with the von Neumann stability analysis we require that amplitudes of Fourier-components be not amplified, that is if we require

\[
|G_{\text{Lax}}(\alpha, \theta)| \leq 1 \text{ for all } \theta
\] (9.5)

we obtain the stability conditions indicated in section 6 (see P.J. Roache, 1972, pp. 42-45). For a time interval of length \(\lambda\Delta t / \Delta x\), which we keep fixed when refining the grid spacing \(\Delta t\) and \(\Delta x\), the relative total error

\[
|G_{\text{Lax}}^{\lambda/\Delta x} - G^{\lambda/\Delta x}| / |G^{\lambda/\Delta x}|
\] (9.6)

and the relative phase error

\[
(\arg G_{\text{Lax}} - \arg G) / \arg G
\] (9.7)

may be calculated as a function of the number \(\lambda / \Delta x\) of grid points per wavelength. Analogously we analyze some methods else. One can show that in the nonscalar case \(\lambda \Delta t / \Delta x\) is the time needed for a full oscillation of the Riemann invariant type quantity with greatest propagation speed \(\gamma_{\text{max}}\) to pass some point fixed in space provided that \(\Delta t = \Delta x / |\gamma_{\text{max}}|\).

Plots of the propagating step function together with plots of relative total errors and relative phase errors are shown in Figs. 4 until 6 for explicit methods with Courant-numbers \(\alpha = 0.1 (\cdots), 0.3 (\cdots -), 0.5 (-\cdots), 0.7 (-\cdots -), 0.9 (--\cdots), \) and in Fig. 7 for implicit methods with Courant-numbers \(\alpha = 0.1 (\cdots), 0.5 (-\cdots -), 0.9 (-\cdots -), 1.3 (-\cdots -), 1.7 (--\cdots--).\)
These plotts exhibit the following features:

- The mesh methods of characteristics (Fig. 4) show phase lag for small Courant-numbers and phase advance for large Courant-numbers with methods of odd order (Figs. 4.1 and 4.3) and conversely with the even order method (Fig. 4.2). There is absolutely no overshoot for the first order method (Fig. 4.1) and small overshoot for the higher order methods (Figs. 4.2 and 4.3). In order to get an accuracy of 1% nearly 500 grid points per wave-length are necessary with the first order method, whereas the higher order methods require 15.

Note that the increase of error with grid-number higher than 100 is due to rounding errors. To provoke this effect coefficients have been stored in single precision on an IBM 370 with almost six decimal digits only. The essential calculations however have been done with double precision.

- The family of Lax-Wendroff type methods (Fig. 5) shows phase advance with odd order and phase lag with even order methods. The first order method of Lax (Fig. 5.1) shows no overshoot, whereas the higher order methods produce considerable overshoot, in particular the even order methods (Figs. 5.2 and 5.4) with low Courant-numbers and the odd order method (Fig. 5.3) with high Courant-numbers. For an accuracy of 1% the first order method requires more than 1000 grid points per wavelength, the higher order methods need only 30 to 10.

- The hopscotch-method with large damping (Fig. 6.1) is only first order accurate but shows very small overshoot. Small or no damping leads to improved accuracy at the cost of highly increased overshoot. (Figs. 6.2 and 6.3). Leap-frog seems to produce not as much overshoot if started with the method of Lax-Wendroff (Fig. 6.4).

- All implicit methods discussed here (Fig. 7) produce large overshoot. The fully implicit and the Crank-Nicholson method show phase lag, the centered difference method shows phase advance with Courant-numbers smaller than 1 and phase lag with Courant-numbers greater than 1. With all three methods accuracy improves with small Courant-numbers.
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Step-function propagating over ten time steps
Über zehn Zeitschritte sich fortbewegende Schrittfunktion

Relative total errors at time $\lambda \Delta t/\Delta x$
Relative Gesamtfehler zum Zeitpunkt $\lambda \Delta t/\Delta x$

Relative phase errors; left scale for positive values (+), right scale for negative values (−)
Relative Phasenfehler; linke Skala für positive Werte (+), rechte Skala für negative Werte (−)

4.1 Courant-Isaacson-Rees
4.2 Fromm
4.3 Leonard's «QUICKEST» method

Fig. 4: Results from problems (A) and (B) obtained by mesh-methods of characteristics.

Bild 4: Resultate von Problem (A) und (B) erhalten mit Hilfe von Maschen-Charakteristiken-Methoden.
Fig. 5: Results from problems (A) and (B) obtained by Lax-Wendroff type methods.

Bild 5: Resultate von Problem (A) und (B) erhalten mit Hilfe von Lax-Wendroff-artigen Methoden.
Fig. 6: Results from problems (A) and (B) obtained by hopscotch and leap-frog.
Bild 6: Resultate von Problem (A) und (B) erhalten mit Hilfe von Hopscotch und Leap-Frog.
Fig. 7: Results from problems (A) and (B) obtained by implicit finite difference methods.

Bild 7: Resultate von Problem (A) und (B) erhalten mit Hilfe impliziter Differenzenmethoden.
In order to find out the most economic method we consider attainable accuracy at fixed time $\lambda \Delta t/\Delta x$ as a function of computing effort measured by the number $N$ of evaluations of $F(W)$ necessary to calculate the solution on a length $\lambda$ of the $x$-axis (Fig 9). In order to do this the solution has to be calculated on $(\lambda/\Delta x)^2$ grid points in the $(x,t)$-plane. If $N_f$ is the number of evaluations of $F(W)$ per grid point then $N$ follows from

$$N = \left(\frac{\lambda}{\Delta x}\right)^2 N_f$$  \hspace{1cm} (9.8)

Fig. 8: Grid points within the rectangle $0 \leq x \leq \lambda$ and $0 \leq t \leq \lambda \Delta t/\Delta x$, to be considered for measuring the computing effort.

Bild 8: Gitterpunkte innerhalb des Rechtecks $0 \leq x \leq \lambda$ und $0 \leq t \leq \lambda \Delta t/\Delta x$, welche bei der Messung des Rechenaufwandes betrachtet werden.

Values of $N_f$ are summarized for explicit finite difference methods in the following table:

<table>
<thead>
<tr>
<th>Order</th>
<th>Method</th>
<th>$N_f$ of evaluations of $F(W)$ per grid point</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Lax ($\omega = 2$)</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>Lax-Wendroff two-step</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>Lax-Wendroff one-step</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>leap-frog</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>hopscotch ($\omega = 0$)</td>
<td>0.5</td>
</tr>
<tr>
<td>3</td>
<td>Rusanov-Burstein-Mirin ($\omega = 2$)</td>
<td>3</td>
</tr>
<tr>
<td>4</td>
<td>Abarbanel-Gottlieb-Turkel</td>
<td>4</td>
</tr>
</tbody>
</table>
Attainable accuracy as a function of computing effort as defined above is plotted in Fig. 9 for the family of Lax-Wendroff type methods (LAX = Lax, LW2 = two-step Lax-Wendroff, RBM = Rusanov-Burstein-Mirin, AGT = Abarbanel-Gottlieb-Turkel, LW1 = one-step Lax-Wendroff), for leap-frog (= LF) and hopscotch (= HS). From this we draw the conclusion that for an accuracy of 10% down to 1% most frequently required in practical calculations
- the method of Lax is rather inefficient,
- the method of Rusanov-Burstein-Mirin performs not much better than the method of Lax-Wendroff (see also P. Wesseling, 1973, pp. 19–20), and
- the method of Abarbanel-Gottlieb-Turkel seems to be the most efficient method considered here.

Fig. 9: Attainable accuracy versus computing effort measured in number of evaluations of $F(W)$ for the methods of Lax (LAX), Rubin-Burstein-Mirin (RBM), two-step Lax-Wendroff (LW2), one-step Lax-Wendroff (LW1), leap-frog (LF), hopscotch (HS), and the method of Abarbanel-Gottlieb-Turkel (AGT).

Bild 9: Erreichbare Genauigkeit in Abhängigkeit vom Rechenaufwand gemessen in Aufrufen der Funktion $F(W)$ für die Methoden von Lax (LAX) und Rubin-Burstein-Mirin (RBM), für die ein- und zweistufige Methode von Lax-Wendroff (LW1 bzw. LW2), für Leap-Frog (LF), Hopscotch (HS) und die Methode von Abarbanel-Gottlieb-Turkel (AGT).

Note that the methods of odd or even order show maximal error with $\alpha = 0$ or $\alpha \sim 0.5$ respectively.

Application of higher order methods like the method of Abarbanel-Gottlieb-Turkel often proves unavailing, because of the difficulty for a proper
treatment of boundary conditions, even if they are approximated with one order lower accuracy thereby not destroying the order of the method (see B. Gustafsson, 1975). Some attractive methods else as leap-frog and hopscotch produce considerable overshoot in case of shocks.

The method of Lax-Wendroff seems to represent a good compromise between simplicity (only three points at time level \( n \) are involved), accuracy, speed and robustness (that is moderate overshoot in case of shocks). Because of its simplicity it can be applied to all points except those on the boundary. Seemingly without loss of overall accuracy boundary points can be handled by a proper adaption of the method of Courant-Isaacson-Rees.

Let us now illustrate overshoot reducing techniques on the basis of the method of Lax-Wendroff. Applied on our test problems they yield results exhibited in Fig. 10, which show the following properties:

- Lax-Wendroff with a large enough second order damping term (\( \omega = 0.5 \)) produces absolutely no overshoot, unless it is unstable (this is the case for \( |\alpha| > 0.866 \)) but is only first order accurate (Fig. 10.1).
- With moderate second order damping (\( \omega = 0.1 \)) overshoot is small but the method is still only first order accurate (Fig. 10.2).
- Full fourth order smoothing (\( \omega = 1 \)) does not destroy order and stability of the method (Fig. 10.3). It reduces overshoot to an amount comparable to the method of Fromm, which in a sense optimally depicts the propagation of discontinuities (see P. Wesseling, 1973, p. 24).
- With the method of flux-correction (Fig. 10.4) overshoot is completely removed for Courant-numbers not too large (in fact for \( |\alpha| \leq 0.866 \)). Phoenical flux-correction as proposed by Book, Boris and Hain changes phase properties. There is phase lag for small Courant-numbers and phase advance for large Courant-numbers. Stability is somewhat reduced (in fact to \( |\alpha| \leq 0.707 \)).

Last of all let us compare CPU-time requirements for one-dimensional unsteady flow calculations reported by several authors. CPU-times are summarized in the following table for the following methods:

- the method of characteristics of first order (C1),
- the mesh method of characteristics of first order (MC1), essentially the method of Courant-Isaacson-Rees,
- two-step Lax-Wendroff (LW2) or equivalently the method of Lerat-Peyret (used by Ehlich-Kruse-Stark),
- one-step Lax-Wendroff (LW1),
- leap-frog (LF) with second order smoothing (\( \omega = 0.15 \)), and
- the centered difference method (CD).

\(^2\) There is a variant of flux-correction, which does not alter phase properties nor stability (H. Niessner and T. Bulaty, 1979).
10.1 Second order damping term with $\omega = 0.5$

10.2 Second order damping term with $\omega = 0.1$

10.3 Fourth order smoothing with $\omega = 1$

10.4 Phoenical flux-correction

Fig. 10: Results from problems (A) and (B) obtained by the method of Lax-Wendroff with modifications to reduce overshoot.

Bild 10: Resultate von Problem (A) und (B) erhalten mit Hilfe der Methode von Lax-Wendroff mit Modifikationen zur Reduktion der Überschwingungen.
10. Literature


Zehnder, G. (1971), Berechnung von Druckwellen in der Aufladetechnik. BBC-Mitteilungen 58: 172–176 (there is also an English and a French version of this paper).


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