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THE DESIGNING APPROACH OF DIFFERENCE SCHEMES BY CONTROLLING THE REMAINDER-EFFECT

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SUMMARY

In this paper, based on the idea of the 'modified partial differential equation', a new designing approach to explicit finite difference schemes for the Burgers equation and PDE is proposed. The approach differs from other constructured methods in such a way that it considers the requests of the numerical dissipation and dispersion coefficients first. This method is much more constructional and directional. The results of numerical tests indicate that the method is quite successful. Copyright © 1999 John Wiley & Sons, Ltd.

KEY WORDS: finite difference schemes; differential equations; remainder-effect

1. INTRODUCTION

There are a lot of papers [1–4] discussing the design of finite difference schemes (FDS) by the await-definiting coefficient method. No doubt these methods were successful in constructing an FDS and in seeking the numerical simulations, and were constructional and directional compared with other methods. However, with these methods it is not yet possible to touch deeply upon the advanced problems of FDS, and they are either not strict enough or too complex. Especially, how to control the numerical remainder-effect, such as the numerical dissipation or dispersion of FDS [2,5–7], has not been discussed.

In this paper, based on the idea of the 'modified partial differential equation' of FDS [8], according to the consistency, monotonicity or positivity, the remainder-effect analysis of FDS [5–7], the coefficients of FDS can be determined. So the approach is much more constructional and directional. Moreover, it is a designing way for the high resolutional and high-order accuracy FDS.

In Section 2, some preliminary remarks are introduced. Especially, the modified partial differential equation (MPDE) of FDS and the remaindereffect analysis of FDS are outlined. In Section 3, the case of the non-viscosity Burgers equation is discussed. In particular, a new scheme—the $\mathrm{LW}+\varepsilon$ scheme—is designed. In Section 4, the FDS for the Burgers equation are discussed and analysed. In addition, it is noted that many schemes suited to non-viscosity Burgers equation, such as upwind, Lax, $\mathrm{LW}+\varepsilon$, may be used to numerically compute general Burgers equation. Finally, some discussions and explanations are given. In this paper, the numerical results for non-viscosity Burgers equations are satisfactorily given.

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2. PRELIMINARY REMARKS

Consider the following partial differential equation

$$u_t = Lu, \quad L = L\left(\frac{\partial}{\partial x}\right), \tag{2.1}$$

where x, t, u are the space and time-independent and -dependent variables respectively. L is the space linear partial differential operator depending on $D_x = \partial/\partial x$. Without losing generality, the suitable FDS consistent with (2.1) can be expressed as [1,2]

$$\sum_\alpha A_\alpha u_{j+\alpha}^{n+1} = \sum_\beta B_\beta u_{j+\beta}^n, \tag{2.2}$$

where A_α, B_β are the coefficients of the FDS, α and β take some positive or negative integers depending on the FDS; u_j^n is the numerical approximation of the continuous variable $u(x, t)$ at the grid point (x_j, t_n).

By expanding the scheme in Taylor series at the grid point (x_j, t_n), we have

$$\sum_\alpha A_\alpha \sum_{n=1} \frac{1}{n!} (\Delta t D_t + \alpha\, \Delta x D_x)^n \cdot u_j^n = \sum_\beta B_\beta \sum_{n=1}^{\infty} \frac{(\beta \Delta x)^n}{n!} D_x^n u_j^n, \tag{2.3}$$

where Δt and Δx are the time and space step lengths of the finite difference grid. Using the modified equation approach described by Warming and Hyett, and eliminating the high-order (≥ 2) time derivative terms, we can obtain 'the modified partial differential equation' [8] completely equivalent to the scheme (2.2) as follows:

$$U_t = LU + R_s(U) + R_p(U). \tag{2.4a}$$

Here the superscripts 'n' and subscripts 'j' are omitted. Where the numerical dissipation remainder $R_p(U)$ and the numerical dispersion remainder $R_p(U)$ of the scheme (2.2) respectively are

$$R_s(U) = v_2 \frac{\partial^2 U}{\partial x^2} + v_4 \frac{\partial^4 U}{\partial x^4} + \cdots, \tag{2.4b}$$

$$R_p(U) = \mu_3 \frac{\partial^3 U}{\partial x^3} + \mu_5 \frac{\partial^5 U}{\partial x^5} + \cdots. \tag{2.4c}$$

Based on the analysis and discussion of References [2–8], we have the following conclusions:

1. The consistency condition is

$$\sum_\alpha A_\alpha = \sum_\beta B_\beta. \tag{2.5a}$$

In particular, if $A_\alpha = 0$ $(\alpha \neq 0)$, $A_0 = 1$, then

$$\sum_\beta B_\beta = 1, \tag{2.5b}$$

and if

$$B_\beta > 0, \tag{2.5c}$$

then the scheme is a monotonic and positive scheme, or a TVB (total variation bounded) scheme and non-oscillatory scheme.

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2. If

$$\nu_2 > 0 \quad \text{or} \quad \nu_2 = 0 \quad \text{and} \quad \nu_4 < 0, \tag{2.6a}$$

the scheme (2.2) is numerical dissipative and stable. On the other hand, if

$$\nu_2 < 0 \quad \text{or} \quad \nu_2 = 0 \quad \text{and} \quad \nu_4 > 0, \tag{2.6b}$$

the scheme (2.2) is numerical anti-dissipative and unstable.

3. If

$$\nu_2 = 0, \quad 4|\mu_3| \gg |\nu_4^2|, \tag{2.7}$$

then the scheme (2.2) is numerical superior-dispersive. In the numerical simulation for discontinuous problems (such as shock), the parasitic oscillation or spurious wave may be produced and developed.

From the above discussion, an important problem is proposed here, i.e. how to design a stable, high resolutionary scheme by controlling the numerical effects of dissipation and dispersion.

3. THE DESIGN AND ANALYSIS OF THE FDS FOR NON-VISCOSITY BURGERS

3.1. General case for a two-level explicit scheme

Consider the simple model—non-viscosity Burgers equation:

$$u_t + au_x = 0 \quad (a > 0). \tag{3.1}$$

Note that simple explicit schemes consistent with (3.1) have the following form:

$$u_j^{n+1} = a_1 u_{j+1}^n + a_0 u_j^n + a_{-1} u_{j-1}^n. \tag{3.2}$$

By the Taylor expanding method we have

$$\left(1 + \Delta t D_t + \frac{\Delta t^2}{2!} D_t^2 + \cdots\right) u_j^n$$
$$= \left[(a_1 + a_0 + a_{-1}) + \Delta x (a_1 - a_{-1}) D_x + \frac{\Delta x^2}{2!}(a_1 + a_{-1}) D_x^2 + \frac{\Delta x^3}{3!}(a_1 - a_{-1}) D_x^3 + \cdots\right] u_j^n,$$

or by rewriting it as

$$\left\{[1 - (a_1 + a_0 + a_{-1})] + \Delta t D_t - \Delta x (a_1 - a_{-1}) D_x + \frac{\Delta t^2}{2!} D_t^2 - \frac{\Delta x^2}{2!}(a_1 + a_{-1}) D_x^2 + \cdots\right\} u_j^n$$
$$= 0.$$

Based on (2.5) and the equivalence with the original PDE (3.1), we have

Theorem 1

Assume that the solution $u(x, t)$ of (3.1) be smooth enough, and the scheme (3.2) be consistent with the original PDE (3.1), then

1) $a_1 + a_0 + a_{-1} = 1,$ (3.3a)

$$2)\ a_{-1} - a_1 = c = \frac{a\,\Delta t}{\Delta t} > 0. \tag{3.3b}$$

Denoting $\alpha = 2a_1 + c$, the expression can be rewritten as

$$\left\{D_t + aD_x + \frac{\Delta t}{2} D_t^2 - \frac{\Delta x}{2}\frac{a\alpha}{c} D_x^2 + \frac{\Delta t^2}{3!} D_t^3 + \frac{\Delta x^2}{3!} aD_x^3 + \frac{\Delta t^3}{4!} D_t^4 - \frac{\Delta x^3}{4!}\frac{ax}{c} D_x^4 + \cdots\right\}U = 0. \tag{3.4}$$

Eliminating the high-order time derivations $(\Delta t^n/n!)D_t^n$ $(n \geq 2)$ by the self-elimination method (do not replace with the original equation! Otherwise the resulting MPDE will not be completely equivalent to the original FDS (3.2)!) we can get the MPDE of (3.2)

$$\left\{D_t + aD_x + \frac{\Delta x}{2}\frac{a}{c}(c^2 - \alpha)D_x^2 + \frac{\Delta x^2}{12} a(4c^2 + 2 - 6\alpha)D_x^3 \right.$$
$$\left. + \frac{\Delta x^3}{24}\frac{a}{c}[3\alpha^2 - (12c^2 + 3)a + 6c^4 + 4c^2]D_x^4\right\}U = 0 \tag{3.4b}$$

and rewrite it in the following remainder form

$$U_t + aU_x = R_s(U) + R_p(U), \tag{3.5}$$

$$R_s(U) = \frac{\Delta x}{2}\frac{a}{c}(\alpha - c^2)U_{xx} - \frac{\Delta x^3}{24}\frac{a}{c}[6c^4 + 4c^2 + 3\alpha^2 - (12c^2 + 1)\alpha]U_{xxxx} + \cdots,$$

$$R_p(U) = \frac{\Delta x^2}{12} a(6\alpha - 4c^2 - 2)U_{xxx} + \cdots.$$

Based on the discussion in Section 2, we have

Theorem 2
Assuming that the solution function $u(x, t)$ is smooth enough, and the space step length Δx is small enough, we have

1) if

$$v_2 > 0 \quad \text{or} \quad v_2 = 0 \quad \text{and} \quad v_4 < 0,$$

i.e.

$$a_1 > \frac{c^2 - c}{2} \quad \text{or} \quad a_1 = \frac{c^2 - c}{2} \quad \text{and} \quad c < 1, \tag{3.6a}$$

then the scheme (3.2) is stable and dissipative. On the other hand, if

$$a_1 < \frac{c^2 - c}{2} \quad \text{or} \quad a_1 = \frac{c^2 - c}{2} \quad \text{and} \quad c > 1, \tag{3.6b}$$

then the scheme (3.2) is unstable and anti-dissipative.

2) if

$$a_1 > 0, \tag{3.7}$$

then the scheme (3.2) is monotonic and positive.

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Proof
Following Hirt [9], Warming and Hyett [8] and the discussion in Section 2, the stability of the scheme (3.2) can be safeguarded by the positive condition of the second-order remainder, i.e.

$$v_2 = \frac{a\,\Delta x}{2c}\,(\alpha - c^2) > 0,$$

where $c = a\,\Delta t/\Delta x$ is the Courant number, or

$$\alpha - c^2 = 2a_1 + c - c^2 > 0,$$

or

$$a_1 > \frac{c^2 - c}{2},$$

if $a_1 = (c^2 - c)/2$, then the stable condition is

$$v_4 = \frac{\Delta x^3}{24}\frac{a}{c}\,[6c^4 + c^2 + 3a^2 - (12c^2 + 1)\alpha] > 0$$

because $a, c > 0$ and $\alpha = 2a_1 + c$, then

$$3c^2(1 - c^2) > 0,$$

or

$$c < 1. \tag{3.8}$$

This is the famous CFL condition. The conclusion 2) can be proved in the similar way.

Since $a_1 > 0$, $1 > c > 0$, $a_{-1} = a_1 + c > 0$ and $a_0 = 1 - (2a_1 + c) = 1 - \alpha > 0$, then the scheme (3.2) is monotonic and positive.

3.2. Applications for classical schemes

Based on the remainder expression and theorem 2, we may consider and check a lot of familiar schemes:

$$\text{Upwind: } a_1 = 0 \Rightarrow a_{-1} = c, \quad a_0 = 1 - c, \quad v_2 = \frac{a}{2}(1 - c)\Delta x,$$

$$\mu_3 = -\frac{1}{6}a(1 - c)(1 - 2c)\Delta x^2,$$

$$\text{Lax: } a_1 = \frac{1 - c}{2} \Rightarrow a_{-1} = \frac{1 + c}{2}, \quad a_0 = 0, \quad v_2 = \frac{a}{2c}(1 - c)\Delta x, \quad \mu_3 = \frac{a}{3}(1 - c^2)\Delta x^2,$$

$$\text{FTCS: } a_1 = -\frac{c}{2} \Rightarrow a_{-1} = \frac{c}{2}, \quad a_0 = 1, \quad v_2 = -\frac{1}{2}ca\,\Delta x, \quad \mu_3 = -\frac{a}{6}(1 + 2c^2)\Delta x^2,$$

$$\text{Lax–Wendroff: } a_1 = \frac{c^2 - c}{2} \Rightarrow a_{-1} = \frac{c^2 + c}{2}, \quad a_0 = 1 - c^2, \quad v_2 = 0, \quad v_4 = \frac{ac}{8}(1 - c^2)\Delta x^3,$$

$$\mu_3 = -\frac{a}{6}(1 - c^2)\Delta x^2.$$

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By theorem 2 and the above dissipation and dispersion remainders of every FDS, we have the following result.

Theorem 3
If $u(x, t)$ is smooth enough, Δx is small enough and $c < 1$, then

1. FTCS scheme is unconditionally unstable and anti-dissipative.
2. Upwind, Lax, LW are stable. (Their numerical dissipation curves $v_2 = v(c)$ are shown in Figure 1.)
3. Upwind, Lax are monotonic and positive.
4. LW is not a monotonic, positive and stable scheme.

From the relation (3.3) of theorem 1, we can see that the coefficient a_1 is a key of designing a monotonic and positive explicit scheme. So we must examine the monotonic and positive region of $a_1 = a_1(c)$:

$$\mathscr{D} = \{a_1 = a_1(c) \geq 0,\ 1 > c > 0\}. \tag{3.10}$$

Figure 2 indicates the regions according to the classical schemes of Section 3.2

1. Upwind: $\mathscr{D}_{\mathrm{up}} = \{a_1 = 0,\ 0 < c < 1\}$
2. Lax: $\mathscr{D}_{\mathrm{Lax}} = \{a_1 = (1 - c)/2,\ 0 < c < 1\}$
3. LW: $\mathscr{D}_{\mathrm{LW}} = \{a_1 = (c^2 - c)/2 > 0,\ 0 < c < 1\} = 0$
4. FTCS: $\mathscr{D}_{\mathrm{ftcs}} = \{a_1 = -c/2 > 0,\ 0 < c < 1\} = 0$

Obviously a simple approach to construct a monotonic and positive scheme is to reform the LW scheme by parallel replacement upwards.

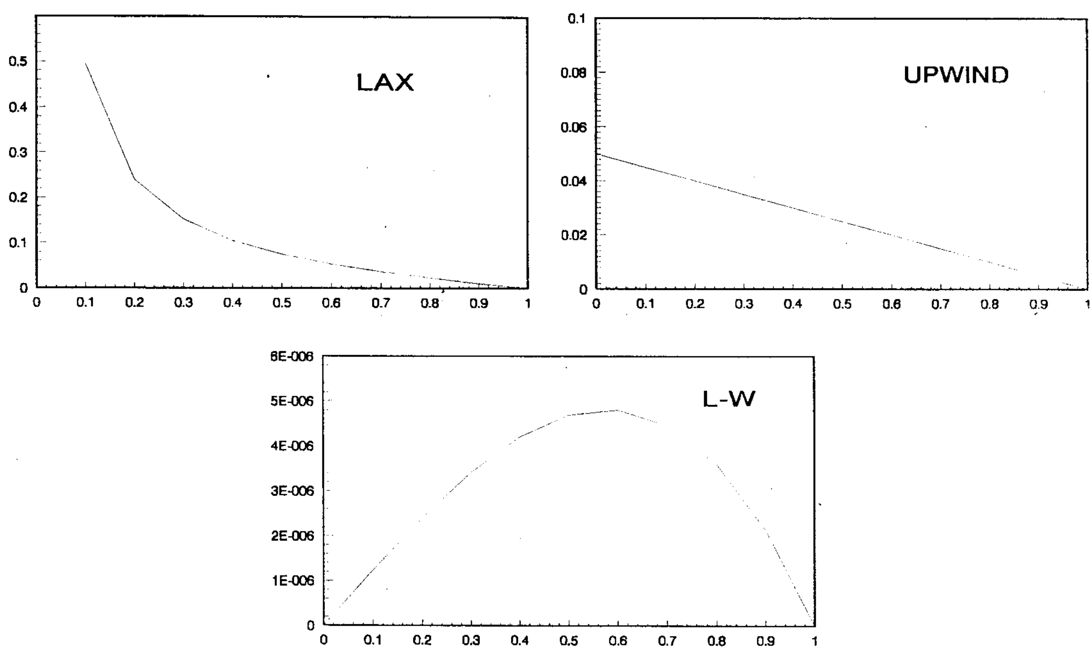

Figure 1. The Lax, the Upwind and the LW numerical dissipation curves $v_2 = v(c)$.

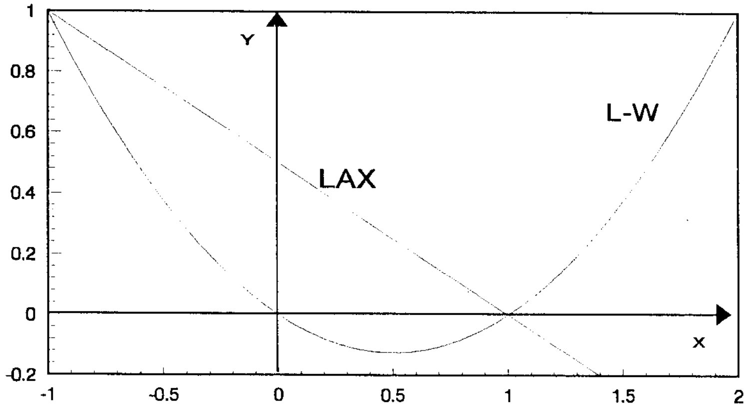

Figure 2. Indication of the regions according to the classical schemes of Section 3.2.

3.3. $LW + \varepsilon$ scheme

Because of the LW scheme's oscillating character and the Lax scheme's 'over smooth' character, we can introduce a new monotonic and positive scheme—the LW + ε scheme—as follows:

$$a_1 = \frac{c^2 + c}{2} + \frac{\varepsilon}{2} \geq 0, \quad \varepsilon = \varepsilon(c) \ll 1 \tag{3.11a}$$

and

$$a_{-1} = \frac{c^2 + c}{2} + \frac{\varepsilon}{2} \geq 0, \quad a_0 = 1 - c^2 - \varepsilon > 0, \tag{3.11b}$$

or

$$u_j^{n+1} = \left(\frac{c^2 - c}{2} + \frac{\varepsilon}{2}\right)u_{j+1}^n + (1 - c^2 - \varepsilon)u_j^n + \left(\frac{c^2 + c}{2} + \frac{\varepsilon}{2}\right)u_{j-1}^n. \tag{3.11c}$$

Obviously, $\varepsilon = \frac{1}{4}$ is a limit case, i.e. the parallel replacement of the parabola of LW's $\mathscr{D}_{\mathrm{LW}}$ to the above c-axis; in this case we have

$$a_1 = \frac{1}{2}\left(c - \frac{1}{2}\right)^2, \quad a_0 = 1 - c^2 - \frac{1}{4}, \quad a_{-1} = \frac{1}{2}\left(c + \frac{1}{2}\right)^2. \tag{3.12a}$$

It is necessary that

$$a_0 = 1 - c^2 - \frac{1}{4} \geq 0, \quad \text{or} \quad c \leq \sqrt{\frac{3}{4}} \doteq 0.8660254, \tag{3.12b}$$

and thus

$$v_2 = \frac{\Delta x}{2}\frac{a}{c}(a - c^2) = \frac{\Delta x}{2}\frac{a\varepsilon}{c} \geq \frac{a\,\Delta x}{4\sqrt{3}}, \tag{3.12c}$$

$$\mu_3 = \frac{\Delta x^2}{12}a(6\alpha - 4c^2 - 2) = \frac{\Delta x^2}{2}a\left(2c^2 - \frac{1}{2}\right) \leq \frac{a\,\Delta x^2}{12}. \tag{3.12d}$$

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Generally speaking, we can take $\varepsilon/2 \geq (c - c^2)/2$, so $a_1 = (c^2 - c)/2 + (\varepsilon/2) \geq 0$, $a_{-1} > 0$, $0 < a_1 \leq 1 - 1/2(c^2 + c)$ and $v^2 \geq (a\,\Delta x/4)(1 - c)$. In this case, the numerical dissipation of the LW + ε scheme is a half that of the Upwind scheme. For example, assuming $a = 1$, $\Delta x = 0.1$, $c = 0.9$, we can take $\varepsilon = 0.1$, thus $a_1 = 0.005$, $a_0 = 0.09$, $a_{-1} = 0.905$, $v_2 = 0.005 < \Delta x^2$, $\mu_3 \doteq 0.0002$. The LW + ε scheme is still second-order-accurate. From the numerical test results given in Figure 3, we can easily see that they are satisfactory.

4. DISCUSSION OF THE EXPLICIT SCHEME FOR BURGERS EQUATION

Now we consider the Burgers equation

$$u_t + au_x = vu_{xx}, \tag{4.1}$$

and still use the three-point explicit scheme (3.2) and the MPDE (3.5).

Theorem 4
Assume that the solution $u(x, t)$ of Burgers equation (4.1) is smooth enough, then the scheme (3.2), consistent with (4.1), satisfies

$$1)\ a_1 + a_0 + a_{-1} = 1, \tag{4.2a}$$

$$2)\ a_{-1} - a_1 = c = \frac{a\,\Delta t}{\Delta x} > 0, \quad c \in (0, 1), \tag{4.2b}$$

$$3)\ v_2 = \frac{\Delta x}{2}\frac{a}{c}(\alpha - c^2) > v \quad \text{or} \quad v_2 = v \quad \text{and} \quad v_4 < 0. \tag{4.2c}$$

By theorem 4, there is an interesting fact that the Upwind scheme, the Lax scheme and the LW + ε scheme may be also effective in numerically simulating the Burgers problems so long as the conditions (4.2) are satisfied. This is the reason that the numerical dissipation of these schemes are enough to replace the real viscosity 'vu_{xx}'. For example, in the case of $a = 1$, $v = 0.01$, $\Delta x = 0.1$, we take $c = 0.795$ for the Upwind scheme, $c = 0.9$ for the Lax scheme and $c = 0.9$, $\varepsilon = 0.18$ for the LW + ε scheme. The numerical results are presented in Figure 4. Obviously the results are satisfactory.

Theorem 5
If $u(x, t)$ is smooth enough and $0 < c < 1$, then

1) The sufficient monotonic and positive condition of the scheme (3.2) for Burgers problems is

$$\sigma = \frac{v\,\Delta t}{\Delta x^2} \in \left[\frac{c - c^2}{2}, \frac{1 - c^2}{2}\right]. \tag{4.3}$$

2) The stability condition is

$$a_1 > \frac{vc}{a\,\Delta x} + \frac{c^2 - c}{2} \tag{4.4a}$$

or

$$a_1 = \frac{vc}{a\,\Delta x} + \frac{c^2 - c}{2} \quad \text{and} \quad c^2 + 6\sigma < 1. \tag{4.4b}$$

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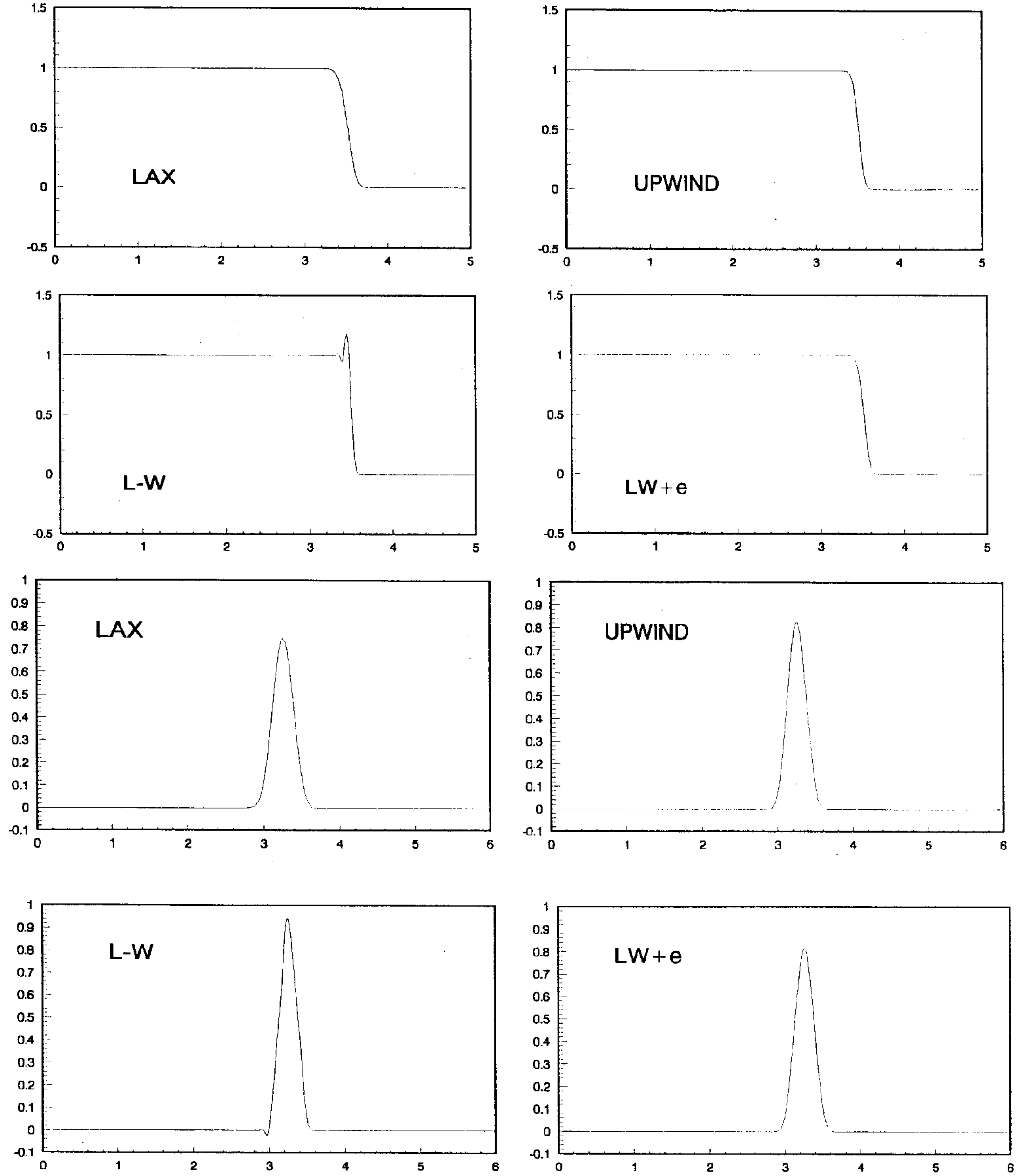

Figure 3. The numerical results of the following problems: (a) $u_t + u_x = 0,\ u(x, 0) = \begin{cases} 1.0, & \text{as } x \le 0 \\ 0.0, & \text{as } x > 0 \end{cases}$. (b) $u_t + u_x = 0,\ u(x, 0) = \begin{cases} 1 - |1 - 2x| & \text{as } 0 < x \le 1.0 \\ 0.0 & \text{otherwise} \end{cases}$.

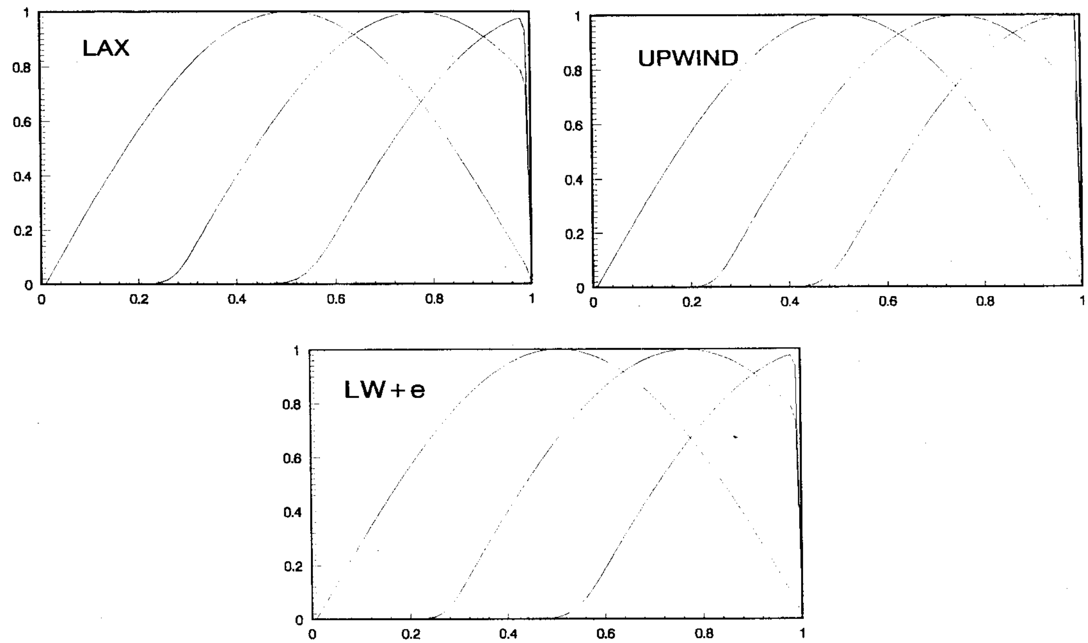

Figure 4. The numerical results of the following problem: $u_t + u_x = \frac{1}{100}u_{xx}$, $u(x, 0) = \sin \pi$, $u(0, t) = u(1, t) = 0$.

Proof

1) Following the discussion in Section 2, from the requirements a_1, a_0 and $a_{-1} > 0$, the condition (4.3) is obvious. Similarly,

2) By theorem 4 or condition (4.2c), (4.4) is also easily introduced.

5. CONCLUSIONS

From this paper we can easily find that the intrinsic characteristics of the schemes mainly depend on the coefficients a_i, $i = -1, 0, 1$ and the Courant number c. Their values greatly influence the schemes' effect of numerical dissipation and dispersion and group velocity. Therefore, a good approach for their selection is to examine the corresponding MPDE form and the remainder-effect of the finite difference schemes, i.e. to suitably control dissipation and dispersion remainders.

We have discussed the simplest two-level explicit schemes, such as the LW, the Upwind and the Lax. In particular, it is well-known that the LW scheme is not monotonic or positive. Besides, it usually introduces non-linear instability. Therefore, we proposed the LW + ε scheme, which overcomes the non-monotonicity. However, how to select ε according to the viscosity ν of Burgers equation is very elaborate.

As far as the general explicit–implicit schemes of Burgers equation is concerned, although they are more difficult than the above simple explicit schemes, a similar approach is still able to achieve success. We will discuss them later in a forthcoming paper.

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