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High Order Difference Schemes for Unsteady One-Dimensional Diffusion–Convection Problems

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For unsteady 1 D diffusion–convection problems, this paper develops an extensive analysis of two-level three-point finite difference schemes of order 2 in time and 4 in space. This general class of FDS includes several schemes independently proposed by different authors. One main objective is the identification of difference schemes yielding satisfactory numerical results for strongly convective problems (i.e., when the cell Reynolds number $\alpha = \lambda h/2$ is greater than unity). The stability and the oscillatory behaviour of the schemes are carefully studied and the analyses are completed by some numerical experiments. We outline some key points: (i) the great difficulty to obtain accurate numerical results for large values of α; (ii) the possibility of virtually optimum schemes is essentially theoretical and requires, in practice, careful experiments; (iii) for strongly convective problems, some second-order explicit schemes are almost as efficient (and less costly) than implicit fourth-order schemes.

1. INTRODUCTION

Our previous paper [1, 2] are concerned with two- and three-level second-order difference schemes (FDS) for the model diffusion–convection problem ($\mathscr{P}$):

$$(\mathscr{P}) \quad \begin{cases} \bullet\ \partial_t u = \partial_x^2 u - \lambda \partial_x u + f = Au + f \quad \text{in }]0, 1[\times [0, T[\\ \bullet\ u(x, 0) = u_0(x), \text{ initial condition for } x \in [0, 1] \\ \bullet\ u = k_i, \text{ boundary conditions for } x_i = 0, 1 \text{ and } t \in [0, T[. \end{cases} \tag{1}$$

These papers outline the importance of an extensive analysis of the properties of the schemes. Beyond the fundamental properties, stability and consistency, the positivity, the numerical dispersion and diffusion must be precisely analysed so as to obtain accurate numerical results, i.e., these which are neither oscillatory nor excessively damped; the artificial viscosity and the positivity of the schemes are of major importance, in particular, for the most interesting problems, i.e., when the convection velocity is high: $\lambda \gg 1$. In [1, 2] we considered most of the first- and second-order schemes and in the present paper we examine higher order schemes (i.e., of order 2 in time and 4 in space) which only need three points in space so as to avoid difficulties near the boundaries.

Recently, several authors have proposed high order, two-level, three-point implicit schemes, e.g., Ciment *et al.* [3], Dennis and Hudson [4] (compact schemes), Iyengar and Mittal [5], Iyengar, Manohar, and Krishnaiah [6], Noye [7]. The optimal weighted scheme given by Richtmyer and Morton [8] is also of order (2, 4). One objective of these works is a satisfactory resolution of linear variable coefficient parabolic equations such as the heat equation in polar cylindrical coordinates.

The purpose of this paper is the utilization of high order schemes for the model problem ($\mathscr{P}$) when the convection velocity is high (without loss of generality, we consider $f \equiv 0$ in the following). With this aim in view, we develop a general approach which includes, as particular cases, most of the schemes already proposed in the papers quoted above. The main characteristic of discrete problems (P_h) associated with ($\mathscr{P}$) is the cell Reynolds number $\alpha = \lambda h/2$. The value $\alpha = 1$ may be considered as a barrier between discrete approximations ($\alpha < 1$) in common use for diffusive problems and those which require a specific approach ($\alpha > 1$). α associates a characteristic of the differential problem, λ, and the space step h; as already noted in [1, 2], we will observe some paradox and conflicts between the asymptotic properties: stability and accuracy, and the behaviour of effective numerical solutions obtained with finite values of the steps Δt, h.

For the construction of the schemes, our process may be compared with the classical *modified equation* technique—Warming and Hyett [9], Sin Chun Chang [10], Noye and Tan [11], Griffiths and Sanz Serna [12] etc. We intend to define the class of two-level three-point schemes of order (2, 4),

$$a_{-1} v_{j-1}^{n+1} + a_0 v_j^{n+1} + a_1 v_{j+1}^{n+1} = b_{-1} v_{j-1}^n + b_0 v_j^n + b_1 v_{j+1}^n, \tag{2}$$

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and obtain as particular cases the following schemes:

— two schemes given by Manohar *et al.* [6];

— the "third-order" scheme given by Noye [7] (this scheme is, in fact, of order 4);

— the optimal weighted scheme of Richtmyer and Morton [8].

Insofar as we consider fourth-order schemes, the numerical dispersion and diffusion will be significantly reduced (at least for moderate values of α). Indeed, they depend on the order of the derivatives appearing in the truncation error or equivalently, on the order of the amplitude and phase errors—see Rigal [1]. Therefore, obtaining stable numerical solutions which do not present oscillations is the main objective of the analysis of the difference schemes.

The presence of non-physical oscillations in the numerical solutions prevents a consistent and stable difference scheme from producing satisfactory numerical results. Different kinds of oscillations may occur—see Siemeniuch and Gladwell [18]; thus, a fundamental necessary condition is the positivity of the FDS, i.e.,

$$\text{for any value of } n\text{: } V^n \geqslant 0 \Rightarrow V^{n+1} \geqslant 0.$$

(This condition is frequently a natural requirement of the physical model).

Let us recall that a matrix $A = [A_{ij}]$ is positive if all its entries a_{ij}, $i = 1, n$ and $j = 1, p$ are positive—this definition is also valid for vectors (n or p equal to unity). Thus, the FDS (2) will be positive if $A^{-1}B$ is a positive matrix, A and B being the tridiagonal matrices $[a_{-1}, a_0, a_1]$ and $[b_{-1}, b_0, b_1]$, respectively.

Unlike second-order schemes, studied in [1], fourth-order schemes are generally not commutative; i.e., the matrices, A and B, do not commute and positivity cannot be easily studied [1, 2, 15].

To discard the FDS which presents roughly oscillatory solutions we defined non-oscillatory schemes [2] as:

DEFINITION. The FDS(2) is non-oscillatory if the associated steady scheme

$$(a_{-1} - b_{-1})\, v_{j-1} + (a_0 - b_0)\, v_j + (a_1 - b_1)\, v_{j+1} = 0 \quad (3)$$

presents monotone solutions.

An FDS which does not satisfy this property will behave as the basic FTCS (forward time, centred space) scheme when $\alpha > 1$. This property, which does not imply the positivity of the scheme, is necessary to obtain satisfactory numerical results over fairly large time intervals. The study of the positivity of the FDS from properties of A and B will be detailed in the next section after the analysis of the fundamental properties, stability and accuracy.

2. CONSTRUCTION AND PROPERTIES OF GENERAL FOURTH-ORDER SCHEMES

We begin with two lemmas relative to two-level three-point schemes (2). We suppose that

$$\sum_{-1}^{1} a_i = \sum_{-1}^{1} b_i = 1,$$

which is always satisfied (after a possible normalization of the coefficients) by consistent schemes.

LEMMA 1. *The FDS(2) is stable if and only if the coefficients a_i, b_i satisfy*

$$(a_1 - a_{-1})^2 - (b_1 - b_{-1})^2 > a_1 + a_{-1} - b_1 - b_{-1} \quad (4)$$

$$(a_1 + a_{-1})^2 - (b_1 + b_{-1})^2 > a_1 + a_{-1} - b_1 - b_{-1}. \quad (5)$$

Proof. The amplification factor associated with (2) is given by

$$g(\varphi) = \frac{b_0 + (b_1 + b_{-1}) \cos \varphi + i(b_1 - b_{-1}) \sin \varphi}{a_0 + (a_1 + a_{-1}) \cos \varphi + i(a_1 - a_{-1}) \sin \varphi}, \quad |\varphi| \in [0, \pi].$$

Taking its modulus, we obtain

$$|g(\varphi)|^2 = 1 - \left(K_1 \sin^2 \frac{\varphi}{2} + K_2 \sin^4 \frac{\varphi}{2}\right) \Big/ D$$

with $D > 0$ and

$$K_1 = 4[(a_1 - a_{-1})^2 - a_1 - a_{-1} + b_1 + b_{-1} - (b_1 - b_{-1})^2]$$

$$K_2 = 16(a_1 a_{-1} - b_1 b_{-1}).$$

The modulus of g will be bounded by unity if

$$K_1 + K_2 Y \geqslant 0 \quad (6)$$

when $Y = \sin^2(\varphi/2)$ describes the interval $[0, 1]$.

The condition (6) will be satisfied if and only if

$$K_1 \geqslant 0, \qquad K_1 + K_2 \geqslant 0, \quad (7)$$

which yields conditions (4) and (5).

LEMMA 2. *The FDS(2) is non-oscillatory if the coefficients a_i, b_i satisfy*

$$(a_1 - b_1)(a_{-1} - b_{-1}) \geqslant 0. \quad (8)$$

Proof. The associated steady scheme (3),

$$(a_1 - b_1)\, v_{j+1} + (a_0 - b_0)\, v_j + (a_{-1} - b_{-1})\, v_{j-1} = 0,$$

is a second-order homogeneous recurrent sequence which will present monotone solutions if the roots of its characteristic equation are real and positive. We may easily verify that the roots are real (recall that $\sum_{-1}^{1} a_i = \sum_{-1}^{1} b_i = 1$) and evidently positive when (8) is satisfied.

With the basic difference operators,

$$D_t v_j^n = \frac{v_j^{n+1} - v_j^n}{\Delta t}, \qquad D_0 v_j^n = \frac{v_{j+1}^n - v_{j-1}^n}{2h},$$
$$D_+ v_j^n = \frac{v_{j+1}^n - v_j^n}{h}, \qquad D_- v_j^n = \frac{v_j^n - v_{j-1}^n}{h}, \tag{9}$$

we define a general two-level three-point scheme (P_h),

(P_h)

$$(1+C)\, D_t v_j^n = (\tfrac{1}{2} + A_1)\, D_+ D_- v_j^n + (\tfrac{1}{2} + A_2)\, D_+ D_- v_j^{n+1} - \lambda(\tfrac{1}{2} + B_1)\, D_0 v_j^n - \lambda(\tfrac{1}{2} + B_2)\, D_0 v_j^{n+1}, \tag{10}$$

where A_i, B_i, C are real constants which must be chosen so as to eliminate lower order terms in the truncation error. When these constants are equal to zero, (P_h) becomes the classical Crank–Nicolson scheme of order (2, 2).

In order to obtain the truncation error, we apply (P_h) to u, a sufficiently smooth solution of $(\mathscr{P}_0)$, the homogeneous problem associated with $(\mathscr{P})$:

$$\begin{aligned} E_u(\Delta t, h) = {} & (1+C)\, D_t u(x_j, t_n) \\ & - (\tfrac{1}{2} + A_2)\, D_+ D_- u(x_j, t_{n+1}) \\ & - (\tfrac{1}{2} + A_1)\, D_+ D_- u(x_j, t_n) \\ & - \lambda(\tfrac{1}{2} + B_2)\, D_0 u(x_j, t_{n+1}) \\ & - \lambda(\tfrac{1}{2} + B_1)\, D_0 u(x_j, t_n); \end{aligned} \tag{11}$$

$u(x, t)$ satisfies

$$\partial_t u + \lambda \partial_x u = \partial_x^2 u \tag{12}$$

and higher order equations which are obtained by differentiating Eq. (12). Thus $E_u(\Delta t, h)$ may be written in terms of the space derivatives only. In the different Taylor developments we retain the terms yielding space derivatives of order up to 6; however, in the coefficients of $\partial_x^5 u$ and $\partial_x^6 u$ we drop the terms depending on Δt^p and h^q with $p > 2$, $q > 4$.

By developing each term in (11) we obtain

$$E_u(\Delta t, h) = \sum_{j=1}^{6} e_j \partial_x^j u + \text{HOD} \quad \text{(higher order derivatives)}$$

with

$$e_1 = \lambda(B_1 + B_2 - C) \tag{13.1}$$

$$e_2 = C - A_1 - A_2 - \lambda^2 \Delta t \left(B_2 - \frac{C}{2}\right) \tag{13.2}$$

$$e_3 = \lambda \left[\Delta t\, (A_2 + B_2 - C) + \frac{h^2}{6}(1 + B_1 + B_2) + \lambda^2 \frac{\Delta t^2}{6}\left[\frac{1}{2} + 3B_2 - C\right]\right] \tag{13.3}$$

$$\begin{aligned} e_4 = {} & \Delta t \left(\frac{C}{2} - A_2\right) - (1 + A_1 + A_2)\frac{h^2}{12} \\ & + \lambda^2 \frac{\Delta t^2}{2}\left(C - \frac{1}{2} - A_2 - 2B_2\right) \\ & - \left(\frac{1}{2} + B_2\right)\lambda^2 \frac{h^2 \Delta t}{6} \\ & + \lambda^4 \frac{\Delta t^3}{24}(C - 4B_2 - 1) \end{aligned} \tag{13.4}$$

$$\begin{aligned} e_5 = \lambda \Bigg[& \frac{\Delta t^2}{2}\left(2A_2 + B_2 + \frac{1}{2} - C\right) \\ & + \frac{h^4}{120}(1 + B_1 + B_2) \\ & + \frac{h^2 \Delta t}{12}\left(\frac{3}{2} + A_2 + 2B_2\right)\Bigg] \end{aligned} \tag{13.5}$$

$$\begin{aligned} e_6 = {} & \frac{\Delta t^2}{2}\left(C - 3A_2 - \frac{1}{2}\right) - (1 + A_1 + A_2)\frac{h^4}{360} \\ & - \frac{h^2 \Delta t}{12}\left(\frac{1}{2} + A_2\right). \end{aligned} \tag{13.6}$$

(P_h) will be of order (2.4), if A_i, B_i, and C are chosen so that the error terms depending on Δt and h^2 vanish in (13.j) for $j = 1, 4$. There is evidently an infinity of solutions: the schemes quoted above [6–8] correspond to different choices which eliminate some other components of the truncation error. In fact it appears that the choice of C only has a slight influence; however, some schemes already proposed correspond to non-null values of C.

Now we shall study the general properties of the class of FDS defined by (10). After that, observing that the schemes previously proposed in [6–8] belong to this class, we complete the analysis of the properties of these schemes and conclude that they are rather poorly efficient for strongly convective problems ($\alpha > 1$). Finally, we examine several choices of the constants A_i, B_i, C so as to propose schemes which may be considered as optimal. From (13.1)–(13.2) we observe

THEOREM 1 (Consistency). (1) *A necessary condition of consistency of* (P_h) *with* $(\mathscr{P})$ *is*

$$C = B_1 + B_2. \tag{14}$$

(2) *(P_h) is consistent with a differential problem with a positive diffusion if the artificial viscosity (characterized by e_2) is less than unity.*

These properties are not important because we will only consider high order schemes, i.e., satisfying at least $e_1 = e_2 = 0$. However, a previous condition must be checked by (P_h); indeed A_i, B_i, C must necessarily be chosen so that (P_h) does not become a backward diffusive scheme. (P_h) will be a forward diffusive scheme if it satisfies the following conditions:

$$\text{(D)} \quad 1 + C > 0, \qquad 1 + A_1 + A_2 > 0. \tag{15}$$

Remark. If (P_h) is formally consistent with a well-posed parabolic problem (P_h) (Theorem 1), conditions (D) seem paradoxical. Insofar as we principally consider strongly convective problems ($\lambda \gg 1$ and $\alpha = \lambda h/2 > 1$), the constants A_i, B_i, and C may be rather large and modify the characteristics of $(\mathscr{P})$. Neither $1 + C$ or $1 + A_1 + A_2$ are considered to be negative (which also corresponds to a forward diffusive scheme), since, in this case, (P_h) approaches $(\mathscr{P})$ with a convective velocity of opposite sign. Actually, this fact points to a major concern of this paper: the asymptotic properties—stability and accuracy—which are obtained for Δt, $h \to 0$, do not always guarantee that the computed solutions of the schemes will be satisfactory. These difficulties (evoked in Section 1) require deeper investigations, particularly for small but finite values of h—see papers [1, 2, 13, 14].

From Lemmas 1 and 2, applied to (P_h), we deduce the following fundamental results.

THEOREM 2 (Stability). *(P_h) is stable if and only if the coefficients A_i, B_i, C and the mesh ratios $r = \Delta t/h^2$, $\mu = \lambda\, \Delta t/h$ verify*

$$\text{(S)} \quad \mu^2(B_1 - B_2) \leqslant 2r(1 + A_1 + A_2), \tag{16}$$

$$2r(A_1 - A_2) \leqslant 1 + C. \tag{17}$$

Proof. This is straightforward from Lemma 1 if we assume that (P_h) satisfies conditions (D). For (P_h) the values of a_i, b_i are given by (in this case $\sum a_i = \sum b_i = 1 + C$):

$$\begin{aligned}
a_0 &= 1 + C + r + 2rA_2, & b_0 &= 1 + C - r - 2rA_1,\\
a_1 &= -\frac{r}{2} - rA_2 + \frac{\mu}{4} + \frac{\mu B_2}{2}, & b_1 &= \frac{r}{2} + rA_1 - \frac{\mu}{4} - \frac{\mu B_1}{2},\\
a_{-1} &= -\frac{r}{2} - rA_2 - \frac{\mu}{4} - \frac{\mu B_2}{2}, & b_{-1} &= \frac{r}{2} + rA_1 + \frac{\mu}{4} + \frac{\mu B_1}{2}.
\end{aligned} \tag{18}$$

THEOREM 3. (Non-oscillation). *(P_h) is non-oscillatory if the following condition* (O) *is satisfied:*

$$\text{(O)} \quad 1 + A_1 + A_2 \geqslant \alpha(1 + C). \tag{19}$$

This condition is deduced from Lemma 2 with the a_i, b_i given by (18) *(we suppose that conditions* (D) *are satisfied).*

3. ANALYSIS OF SOME FOURTH-ORDER SCHEMES

The finite difference schemes analyzed in this section have been introduced independently by different authors. The construction and the objectives of these schemes are quite different but they have in common the utilization of two time levels and of space operators of order at most 2, yielding an accuracy of order (2, 4). They have been proposed for diffusion problems, so their behaviour for convection–diffusion problems when the convection velocity is large must be analysed. With the basic difference operators given in (9) we define four schemes below:

1. *W Scheme*

The optimal weighted scheme given by Richtmyer and Morton [8, p. 188] for the heat equation is adapted to $(\mathscr{P})$ as

$$\begin{aligned}
\text{(W)} \quad D_t v_j^n - (D_+ D_- - \lambda D_0)\left(\frac{v_j^{n+1} + v_j^n}{2}\right)
&= \frac{\lambda^2 h^2}{12} D_+ D_- \left(\frac{v_j^{n+1} + v_j^n}{2}\right) + \frac{\lambda^2 h^2}{12} D_t D_0 v_j^n\\
&\quad - \left(\frac{h^2}{12} + \frac{\lambda^2 h^4}{144}\right) D_t D_+ D_- v_j^n
\end{aligned} \tag{20}$$

or, equivalently,

$$D_t v_j^n = \left[\left(1 + \frac{\lambda^2 h^2}{12}\right) D_+ D_- - \lambda D_0\right] [\theta_0 v_j^{n+1} + (1 - \theta_0)\, v_j^n]$$

with θ_0 the optimal weighting parameter given by

$$\theta_0 = \frac{1}{2} - \frac{1}{12r}.$$

The W-scheme belongs to class (P_h) with the constants:

$$C=0, \qquad B_1=-B_2=\frac{1}{12r},$$
$$A_1=\frac{\lambda^2h^2}{24}+\frac{1}{12r}+\frac{\lambda^2h^2}{144r}, \qquad A_2=\frac{\lambda^2h^2}{24}-\frac{1}{12r}-\frac{\lambda^2h^2}{144r}. \tag{21}$$

2. *N Scheme*

This scheme was obtained by Noye [7] in 1990 from a combination of Lax–Wendroff and backward optimal schemes (the author, surprisingly, declared that the scheme was of order 3):

$$\text{(N)} \quad D_t v_j^n-(D_+D_- -\lambda D_0)\left(\frac{v_j^{n+1}+v_j^n}{2}\right)$$
$$=\left(\frac{\lambda^2h^2}{12}-\frac{\lambda^4\Delta t^2}{12}\right)D_+D_-\left(\frac{v_j^{n+1}+v_j^n}{2}\right)$$
$$+\left(\frac{\lambda h^2}{12}-\frac{\lambda^3\Delta t^2}{12}\right)D_tD_0v_j^n$$
$$-\left(\frac{h^2}{12}+\frac{\lambda^2\Delta t^2}{6}\right)D_tD_+D_-v_j^n. \tag{22}$$

The N scheme corresponds to (P_h) with

$$C=0, \qquad B_1=-B_2=\frac{1}{12r}-\frac{\lambda^2\Delta t}{12},$$
$$A_1=\frac{\lambda^2h^2}{24}-\frac{\lambda^4\Delta t^2}{24}+\frac{1}{12r}+\frac{\lambda^2\Delta t}{6}, \tag{23}$$
$$A_2=\frac{\lambda^2h^2}{24}-\frac{\lambda^4\Delta t^2}{24}-\frac{1}{12r}-\frac{\lambda^2\Delta t}{6}.$$

3. *M1 Scheme*

This scheme and its variant defined below were constructed by Manohar, Iyengar, and Krishnaïah [6] in 1988 for parabolic problems with variable coefficients (in particular, for differential problems in polar coordinates):

$$\text{(M1)} \quad D_tv_j^n-(D_+D_- -\lambda D_0)\left(\frac{v_j^{n+1}+v_j^n}{2}\right)$$
$$=\frac{\lambda^3h^2}{12}D_0\left(\frac{v_j^{n+1}+v_j^n}{2}\right)+\frac{\lambda^2h^2}{12}D_tv_j^n$$
$$+\frac{\lambda h^2}{12}D_tD_0v_j^n-\left[\frac{h^2}{12}-\frac{\lambda^2h^4}{72}\right]D_tD_+D_-v_j^n. \tag{24}$$

The M1 scheme corresponds to (P_h) with

$$C=-\frac{\lambda^2h^2}{12},$$
$$B_1=-\frac{\lambda^2h^2}{24}+\frac{1}{12r}, \qquad B_2=-\frac{\lambda^2h^2}{24}-\frac{1}{12r}, \tag{25}$$
$$A_1=-A_2=\frac{1}{12r}-\frac{\lambda^2h^2}{72r}.$$

4. *M2 Scheme*

Another choice of coefficients made by Manohar *et al.* yields

$$\text{(M2)} \quad D_tv_j^n-(D_+D_- -\lambda D_0)\left(\frac{v_j^{n+1}+v_j^n}{2}\right)$$
$$=\frac{\lambda^2h^2}{6}D_+D_-\left(\frac{v_j^{n+1}+v_j^n}{2}\right)$$
$$-\frac{\lambda^3h^2}{12}D_0\left(\frac{v_j^{n+1}+v_j^n}{2}\right)$$
$$-\frac{\lambda^2h^2}{12}D_tv_j^n+\frac{\lambda h^2}{12}D_tD_0v_j^n$$
$$-\left[\frac{h^2}{12}+\frac{\lambda^2h^4}{72}\right]D_tD_+D_-v_j^n. \tag{26}$$

The M2 scheme corresponds to (P_h) with

$$C=\frac{\lambda^2h^2}{12}, \qquad A_1=\frac{\lambda^2h^2}{12}+\frac{1}{12r}+\frac{\lambda^2h^2}{72r},$$
$$A_2=\frac{\lambda^2h^2}{12}-\frac{1}{12r}-\frac{\lambda^2h^2}{72r}, \tag{27}$$
$$B_1=\frac{\lambda^2h^2}{24}+\frac{1}{12r}, \qquad B_2=\frac{\lambda^2h^2}{24}-\frac{1}{12r}.$$

Replacing the above sets of constants in the expressions (13.j), we obtain the truncation errors relative to every scheme:

$$E_W=\left[\frac{\lambda^3h^4}{144}-\frac{\lambda^3\Delta t^2}{12}\right]\partial_x^3u+\left[\frac{\lambda^2\Delta t^2}{4}-\frac{\lambda^2h^4}{72}\right]\partial_x^4u$$
$$+\left[\frac{\lambda h^4}{80}-\frac{\lambda\Delta t^2}{4}\right]\partial_x^5u$$
$$+\left[\frac{\Delta t^2}{12}-\frac{h^4}{240}\right]\partial_x^6u+\text{HOD} \tag{28}$$

$$E_{\mathrm{N}}=\left[\frac{\lambda^2\,\Delta t^2}{12}-\frac{\lambda^2 h^4}{144}\right]\partial_x^4 u+\left[\frac{\lambda h^4}{80}-\frac{\lambda\,\Delta t^2}{4}\right]\partial_x^5 u$$
$$+\left[\frac{\Delta t^2}{4}-\frac{h^2\,\Delta t}{12}-\frac{h^4}{240}\right]\partial_x^6 u+\mathrm{HOD} \qquad (29)$$

$$E_{\mathrm{M1}}=-\frac{\lambda^3\,\Delta t^2}{12}\partial_x^3 u+\frac{\lambda^2\,\Delta t^2}{4}\partial_x^4 u+\left[\frac{\lambda h^4}{80}-\frac{\lambda\,\Delta t^2}{4}\right]\partial_x^5 u$$
$$+\left[\frac{\Delta t^2}{4}-\frac{h^2\,\Delta t}{12}-\frac{h^4}{240}\right]\partial_x^6 u+\mathrm{HOD} \qquad (30)$$

$$E_{\mathrm{M2}}=-\frac{\lambda^3\,\Delta t^2}{12}\partial_x^3 u+\left(\frac{\lambda^2\,\Delta t^2}{4}-\frac{\lambda^2 h^4}{72}\right)\partial_x^4 u$$
$$+\left(\frac{\lambda h^4}{80}-\frac{\lambda\,\Delta t^2}{4}\right)\partial_x^5 u$$
$$+\left(\frac{\Delta t^2}{4}-\frac{h^2\,\Delta t}{12}-\frac{h^4}{240}\right)\partial_x^6 u+\mathrm{HOD}. \qquad (31)$$

Note that, except for the N scheme, in the expressions above, e_1 and e_2 are the only coefficients equal to zero. Thus, it appears that the choice of A_i, B_i, C may be improved. Now, we give the main results relative to these schemes, i.e., the conditions (D), (S), (O) corresponding to each of them.

THEOREM 4. 1. *The W scheme satisfies conditions* (D) *and* (O) *for any value of* Δt, *h and is stable* (*conditions* (S)) *if*

$$\alpha \leqslant \sqrt{6}. \qquad (32)$$

2. *The N scheme satisfies conditions* (D), (S), *and* (O) *if r is less than* r_1, r_2, r_3, *respectively:*

$$r_1=\frac{1}{2\alpha}\left(1+\frac{3}{\alpha^2}\right)^{1/2} \qquad (33.1)$$

$$r_2=\frac{1}{2\alpha} \qquad (33.2)$$

$$r_3=\frac{1}{2\alpha}\left(1+\frac{3}{\alpha^2}-\frac{3}{\alpha}\right)^{1/2}. \qquad (33.3)$$

3. *The M1 scheme satisfies conditions* (D), (S), *and* (O) *if, respectively,*

(i) $\alpha<\sqrt{3}$ (34.1)

(ii) $\alpha\leqslant\sqrt{6}$ (34.2)

(iii) $\alpha^3-3\alpha-3<0 \Leftrightarrow \alpha<\alpha_1\sim 2.1.$ (34.3)

4. *The M2 scheme satisfies conditions* (D) *and* (S) *for any value of* Δt, *h and condition* (O) *if*

$$\alpha^3-2\alpha^2-3\alpha-3<0 \Leftrightarrow \alpha<\alpha_2\sim 1.4. \qquad (35)$$

The stability results of the M1, M2, N schemes agree with those given by [6, 7], except for the stability domain defined by (41b) in [7] which does not appear in (33). Actually, this condition (41b) may be expressed as

$$r>r^* \quad \text{with} \quad r^*\to\infty \text{ when } h\to 0$$

and is therefore not significant. Besides, the asymptotic behaviour of the above conditions, (32)–(35), will require our attention.

Comments. 1. Several conditions detailed above are independent of Δt, e.g., conditions (34.1)–(34.3) relative to the M1 scheme are always satisfied when h tends to zero. We observe the following paradoxical situation: the Fourier stability analysis which must give an asymptotic result—stability yielding convergence of the discrete scheme following the Lax–Richtmyer theorem [8]—leads to stability conditions (W and M1 schemes) which are only significant when h is finite. Such conditions are crucial for practical computations (finite values of h and $\lambda \gg 1$), but some anomalies do appear: for instance, considering the M1 scheme, it is a backward diffusive scheme when $\alpha>\sqrt{3}$ (conditions (D) non-satisfied) and, therefore, gives numerical solutions which are quite unstable even if $\alpha<\sqrt{6}$ (conditions (S) satisfied).

Briefly, if conditions (D), (S), and (O) are satisfied, we may expect numerical results which are generally satisfactory but not necessarily of order (2, 4). Indeed, the above observations are also valid for the discretization errors which present some coefficients that are dependent on λh; thus these errors may behave like $O(h^2)$ or even $O(h)$. Another limitation to the efficiency of numerical schemes is their non-positivity which we discuss below.

2. The preceding observations do not apply to the N scheme submitted to conditions (33.1)–(33.3) which are of the same kind as those obtained for second-order schemes [1]. No direct limitation of the cell Reynolds number α appears and conditions (33.1)–(33.3) may be interpreted as conditions on the Courant number $\mu=2\alpha r$; e.g., condition (S) is then $\mu\leqslant 1$. Moreover, contrary to (28), (30), (31), the truncation error E_N (29) does not present any term depending on λ^3. Therefore, among these four schemes, the N scheme appears to be the best.

Positivity of the FDS

To achieve the analysis, we consider the positivity of the difference schemes. The matrix formulation

$$AV^{n+1}=BV^n,$$

where A and B are tridiagonal matrices,

$$A=[a_{-1},a_0,a_1], \qquad B=[b_{-1},b_0,b_1], \qquad (36)$$

leads to two cases being distinguished:

(i) if matrices A and B commute—as matrices relative to second-order two-level schemes [1], the FDS may then be interpreted as rational approximation of $\exp(-z)$ and the positivity results from the monotonicity of these approximations [1, 15]. Among the above FDS, the W scheme is the only one that is commutative.

(ii) if matrices A and B do not commute, the positivity of the scheme (defined in Section 1) is then certain if both matrices A^{-1} and B are positive. Let us recall that a nonsingular matrix A is monotone if A^{-1} is positive. No simple characterization of monotone matrices exists. A simple sufficient condition is that A is a diagonally dominant L-matrix (DDL matrix), i.e.,

$$a_{ii} > 0, \qquad a_{ij} \leqslant 0 \qquad \text{if} \quad j \neq i \qquad (L\text{-matrix}) \tag{37}$$

$$a_{ii} \geqslant \sum_{j \neq i} |a_{ij}| \qquad \text{(diagonal dominance).} \tag{38}$$

In our case, we will impose:

$$\begin{aligned} &b_0 \geqslant 0, \qquad b_1 \geqslant 0, \qquad b_{-1} \geqslant 0, \\ &a_0 > 0, \qquad a_1 < 0, \qquad a_{-1} < 0, \qquad a_0 > |a_1| + |a_{-1}|. \end{aligned} \tag{39}$$

The above properties evidently yield sufficient (and frequently too restrictive) conditions. In short, we attempt to propose realistic positivity conditions for comparison with numerical experiments. The experimental limits of positivity are somewhat imprecise because they slightly depend on the data of the differential problem. The positivity conditions are detailed below for the four preceding schemes which are first assumed to verify conditions (D), (S), and (O).

THEOREM 5. *The W scheme is positive if r belongs to the interval*

$$r \in \left[\frac{1}{6}, \frac{15 - \alpha^2}{18 + 6\alpha^2}\right]. \tag{40}$$

Proof. The W scheme may be written

$$(I - \theta\, \Delta t\, Q)\, V^{n+1} = (I + (1 - \theta)\, \Delta t\, Q)\, V^n$$

with $Q = (1 + \lambda^2 h^2/12)\, D_+ D_- - \lambda D_0$ and $\theta = \frac{1}{2} - 1/12r$ and is positive if $R(z) = (1 - (1 - \theta)z)/(1 + \theta z)$ is monotone on $\mathbb{R}^+$[1, 15]. (Note that Q is positive when condition (D) is satisfied). Thus we prescribe:

- $\theta > 0$
- $1 - (1 - \theta)\sup(q_i) > 0$, where $[q_i]$ is the diagonal part of the matrix associated with Q and we obtain (40).

THEOREM 6. *The* M1 *and* M2 *schemes are positive if, respectively,*

$$r < r_{p_1} = \frac{15}{16} - \frac{\alpha^2}{4} \tag{41.1}$$

$$r < r_{p_2} = \frac{15 + 4\alpha^2}{16 + 12\alpha^2}. \tag{41.2}$$

Proof. These conditions result from (38) when we take conditions (D), (S), and (O) into account, i.e.,

$$\alpha \in [0, \sqrt{3}[\qquad \text{for the M1 scheme}$$

$$\alpha \in [0, \alpha_1[\qquad \text{for the M2 scheme.}$$

The positivity results relative to the N scheme are given in [7] in terms of r and $\mu = 2\alpha r$, the Courant number; these results are rather involved and not quite exact. The coefficients a_i, b_i are given by

$$\begin{aligned} a_{-1} &= (1 - 6r - 4\alpha^2 r^2)(2r + 2\alpha r - 4\alpha^2 r^2) \\ a_0 &= 2(12r - (2r - 4\alpha^2 r^2)(1 - 6r - 4\alpha^2 r^2)) \\ a_1 &= (1 - 6r - 4\alpha^2 r^2)(2r - 2\alpha r - 4\alpha^2 r^2) \\ b_{-1} &= (1 + 6r - 4\alpha^2 r^2)(2r + 2\alpha r + 4\alpha^2 r^2) \\ b_0 &= 2(12r - (2r + 4\alpha^2 r^2)(1 + 6r - 4\alpha^2 r^2)) \\ b_1 &= (1 + 6r - 4\alpha^2 r^2)(2r - 2\alpha r + 4\alpha^2 r^2). \end{aligned} \tag{42}$$

We separately examine the positivity of B and A^{-1}.

PROPOSITION 1. *$B = [b_{-1}, b_0, b_1]$ is a positive matrix if*

$$r > r_1^* = \frac{\alpha - 1}{2\alpha^2} \tag{43}$$

and

$$r < \inf\{r_{-1}, r_{0_i}\} \qquad \text{with} \quad r_{-1} = (3 + \sqrt{9 + 4\alpha^2})/4\alpha^2 \tag{44}$$

and r_{0_i} is specified below.

Proof. The conditions $r > r_1^*$ and $r < r_{-1}$ are straightforward from the positivity of b_1 and b_{-1}; $b_0 > 0$ yields the inequality

$$P_\alpha(r) = 8\alpha^4 r^3 - 8\alpha^2 r^2 - 2\alpha^2 r - 6r + 5 > 0 \tag{45}$$

and we must approximate the first positive root r_0 of $P_\alpha(r)$ (which is easy to compute for given values of α). The study of the family of curves associated with P_α gives an estimate of r_0:

$$r_{01}=\frac{45}{2}\frac{(2+\sqrt{13+3\alpha^2})}{[118\alpha^2+70+(26+6\alpha^2)\sqrt{13+3\alpha^2}]}. \quad (46)$$

This value corresponds to the intersection between the r-axis and the straight line joining (0,5) and the first minimum of $P_\alpha(r)$ (i.e., when $r=r_m=(2+\sqrt{13+3\alpha^2})/6\alpha^2$). Moreover, $b_0>0$ is equivalent to

$$(1+2\alpha^2 r)(1+6r-4\alpha^2r^2)<6 \quad (47)$$

and $1+6r-4\alpha^2r^2$ is a maximum in the interval $[0, r_{-1}]$ for $r=3/4\alpha^2$. Thus with this value in Eq. (47) we obtain a sufficient condition,

$$r<r_{02}=\frac{20\alpha^2-9}{2\alpha^2(4\alpha^2+9)}, \quad (48)$$

which is obviously significant only when $\alpha>3/2\sqrt{5}\simeq 0.67$.

PROPOSITION 2. *$A=[a_{-1}, a_0, a_1]$ is an DDL-matrix if*

$$r'<r<r'',$$

where

$$r'=\frac{\sqrt{9+4\alpha^2}-3}{4\alpha^2}, \qquad r''=\frac{1-\alpha}{2\alpha^2}. \quad (49)$$

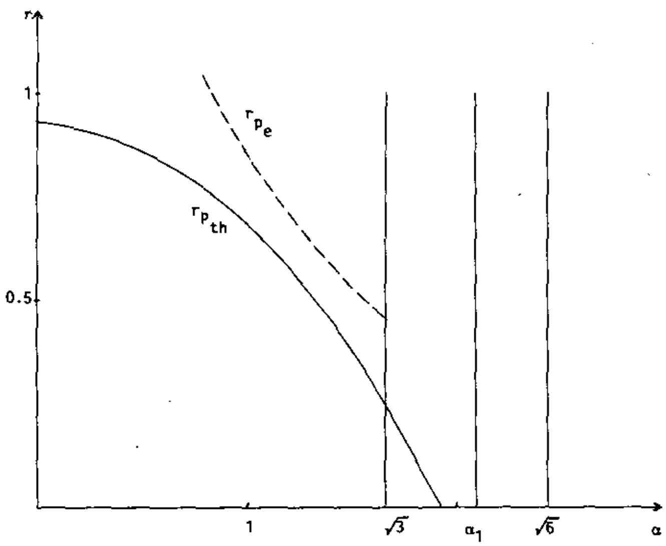

FIG. 1. M1 scheme: $\alpha=\sqrt{3}$, α_1 ($\simeq 2.1$), $\sqrt{6}$ are the limits given by conditions (D), (O), and (S), respectively; $r_{P_{th}}$ and r_{P_e} are the theoretical and experimental positivity limits.

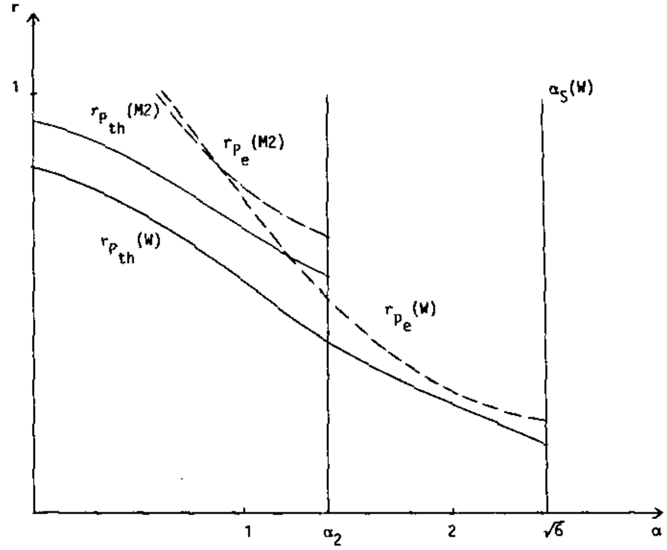

FIG. 2. M2 and W schemes: $\alpha_S=\sqrt{6}$ is the stability limit of the W scheme; $\alpha_2\simeq 1.4$ is the non-oscillation limit of the M2 scheme; $r_{P_{th}}$ and r_{P_e} are the theoretical and experimental positivity limits, respectively.

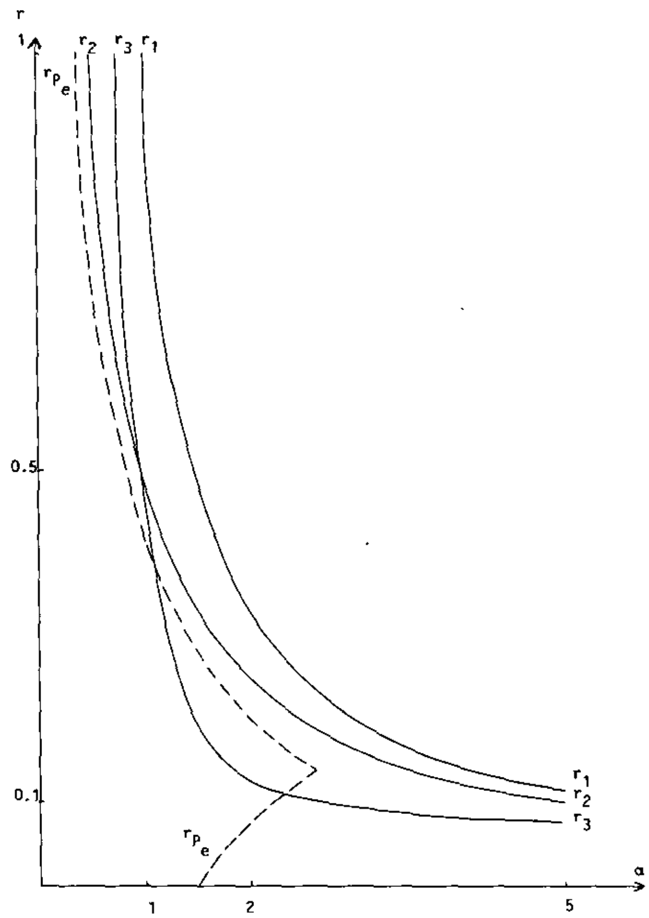

FIG. 3. N scheme: r_1, r_2, r_3 are the limits given by conditions (D), (S), and (O), respectively; r_{P_e} is the experimental positivity limit.

Proof. These conditions result from the negativity of a_1 and a_{-1} which is satisfied under the above conditions. A is then diagonally dominant. Note that the inequalities (49) are never valid if $\alpha \geqslant \frac{4}{5}$.

Conclusion. Both above propositions yield conditions of quite different consequences. Proposition 2 (A is a DDL-matrix) gives widely sufficient conditions which may be very significantly exceeded, while Proposition 1 gives nearly realistic conditions. This situation is common to other schemes, but, for M1 and M2 schemes, the conditions on A are inequalities excluding values of r near zero and therefore are not important.

On Figs. 1–3 we summarize the results relative to the four preceding schemes. The common observation is that they are only efficient for weak or moderate values of α; it is not possible to consider values of α greater than about 1.5 (M1 or M2 scheme) or 2.5 (W or N scheme). However, we distinguish the properties (D), (S), and (O) which must be verified so as not to destroy the numerical solutions and the positivity property which does not prevent the computation of acceptable numerical solutions. Therefore, the N scheme is the only one which does not present a barrier value for α and appears as the most efficient among these four schemes.

There obviously exists an infinity of possible choices of the constants A_i, B_i, C, such that the truncation error will be of order (2, 4). Different possibilities will be discussed in the following paragraph.

4. TOWARDS AN OPTIMAL SCHEME

The discussion is limited to three situations corresponding to different approaches of the discretization error $E_u(\Delta t, h)$ given by (11):

(i) we eliminate the only components of E_u of order strictly lower than 2 in time and 4 in space; thus, we define the R1 scheme;

(ii) we choose the A_i, B_i so as to cancel the four coefficients (e_i) given by (13.1)–(13.4) in E_u and we obtain the R2 scheme;

(iii) we consider the class of R3 schemes defined by a choice of constants which cancel e_1, e_2, e_3 in E_u; in this class (containing the N and R2 schemes) we seek an optimal scheme of order (2, 4) which verifies the fundamental properties and leads to minimal restrictions on grid steps.

Preliminary Remark. In the general formulation (10) of (P_h) we introduced the constant C because the M1, M2 schemes given by Manohar *et al.* [6] correspond to values of C different from zero. In fact, the choice of C (provided that $1 + C > 0$) has no consequences on the basic properties of the schemes. Therefore, the following schemes will be studied with $C = 0$ (which makes the different analyses easier) and we might verify, sometimes with difficulty, that conditions (D), (S), and (O) are independent of C.

However, the amplitude of the discretization error depends on the choice of C (see Eqs. (13.1)–(13.6)). The numerical tests (Section 5) show that this dependence is not very close for transient-state computations, but if we consider the steady-state problem associated with (P_h) (as we introduced condition (O)), it appears from Eq. (10) that the approach of steady-state solutions will be satisfactory only if C is relatively near $A_1 + A_2$. If not, the diffusion of the discrete problem will be very different from that of the differential problem; this difficulty is particulary present in R3 schemes (and confirmed by numerical experiments) because a consequence of the improvement of the properties of the FDS is an increase of the artificial viscoscity.

R1 SCHEME. The constants A_i, B_i satisfying

$$\begin{aligned} B_1 + B_2 &= 0 \\ A_1 + A_2 + \lambda^2 \Delta t\, B_2 &= 0 \\ \Delta t\,(A_2 + B_2) + \frac{h^2}{6} &= 0 \\ (1 + A_1 + A_2)\frac{h^2}{12} + A_2\,\Delta t &= 0 \end{aligned} \tag{50}$$

eliminate the only terms depending on Δt and h^2 in $E_u(\Delta t, h)$ (11). From (50) we deduce that

$$B_2 = -\frac{1}{4r(\alpha^2+3)}, \qquad A_2 = -\frac{(2\alpha^2+3)}{12r(\alpha^2+3)},$$
$$A_1 = -1 - A_2(1+2r), \qquad B_1 = -B_2 \tag{51}$$

and E_u becomes

$$\begin{aligned} E_{R_1} = {} & \frac{\lambda^2 \Delta t^2}{12}(1 + 6B_2)\,\partial_x^3 u \\ & - \left[\lambda^2 \frac{\Delta t^2}{4}(1 + 2A_2 + 4B_2) + \frac{\lambda^2 h^2 \Delta t}{12}(1 + 2B_2)\right]\partial_x^4 u \\ & + \left[\frac{\lambda\,\Delta t^2}{4}(1 + 2B_2 + 4A_2) + \frac{h^4}{120} \right. \\ & \left. + \frac{h^2 \Delta t}{24}(3 + 2A_2 + 4B_2)\right]\partial_x^5 u \\ & - \left[\frac{\Delta t^2}{4}(1 + 6A_2) + \frac{h^2 \Delta t\, A_2}{20} + \frac{h^2 \Delta t}{24}\right]\partial_x^6 u + \text{HOD}. \end{aligned}$$

By applying conditions (15), (17), (19), we obtain

THEOREM 7. *The R1 scheme is stable and non-oscillatory if, respectively,*

$$\text{(i)}\quad r \leqslant r_{s_1} = \frac{1}{6} + \frac{1}{\alpha^2} \qquad\qquad (52)$$
$$\text{(ii)}\quad \alpha < \alpha_2$$

and satisfies conditions (D) *for any* Δt, h.

Proof. Some algebraic calculus yields conditions (52), where α_2 given by (35) is the positive root of

$$\alpha^3 - 2\alpha^2 + 3\alpha - 3 = 0.$$

This scheme does not present any improvement in comparison with the schemes analyzed in Section 3. For completeness, we give the positivity results deduced from the matrix formulation (35) with the a_i, b_i given by (18).

PROPOSITION 1. *B is positive if*

$$r \leqslant r_1 = \frac{4\alpha^2 + 15}{18\alpha^2 + 18}. \qquad (53)$$

Proof. The positivity of b_0 yields (53), b_{-1} is always positive, and b_1 is positive if

$$\alpha \leqslant 1 + \sqrt[3]{2} \qquad \text{or} \qquad r < r_2 = \frac{2\alpha^2 - 3\alpha + 3}{(\alpha - 1)^3 - 2}.$$

However, in the interval of usual values of α, we have $r_1 < r_2$ and the positivity condition of B is (53).

PROPOSITION 2. *A is an DDL-matrix if*

$$\alpha < 1 \qquad \text{and} \qquad r > r^* = \frac{2\alpha^2 - 3\alpha + 3}{6(1-\alpha)(\alpha^2 + 3)}. \qquad (54)$$

Proof. a_0 is always positive, a_1 is negative if (54) is satisfied, and a_{-1} is negative if

$$r > r^{**} = \frac{2\alpha^2 + 3\alpha + 3}{6(\alpha + 1)(\alpha^2 + 3)}.$$

r^{**} is smaller than r^* when $\alpha < 1$; then the only conditions are given by (54). ∎

Figure 4 summarizes these results and clearly outlines that, like the schemes analyzed in Section 3, the R1 scheme does not work efficiently for larger values of α (i.e., greater than about 1.5).

R2 SCHEME. The constants A_i, B_i are chosen so as to

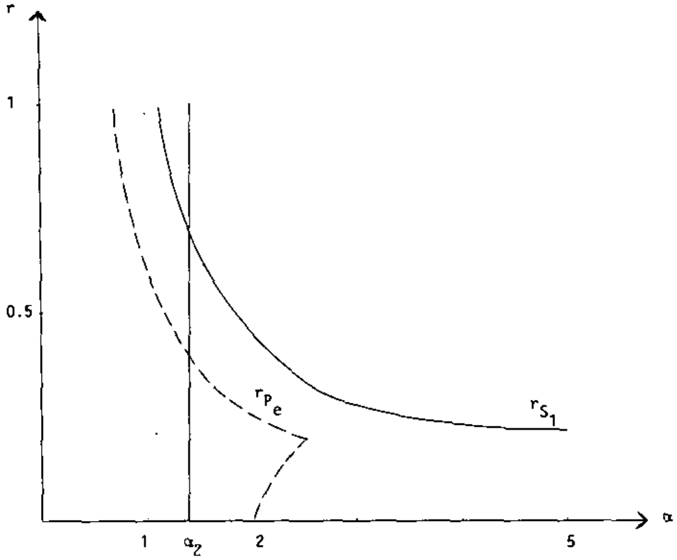

FIG. 4. R1 scheme: r_{s_1}, stability limit (52); r_{P_e}, experimental positivity limits; $\alpha = \alpha_2$ ($\simeq 1.4$) is the limit given by condition (O).

cancel the four coefficients $\{e_i\}_{i=1,4}$ in E_u. Taking C equal to zero, we obtain

$$B_2 = \frac{q}{p}, \qquad B_1 = -B_2$$
$$A_2 = -\frac{\lambda^2 \Delta t}{12} - \frac{1}{6r} - \frac{q}{p} - \frac{q}{p}\frac{\lambda^2 \Delta t}{2} \qquad (55)$$
$$A_1 = \frac{\lambda^2 \Delta t}{12} + \frac{1}{6r} + \frac{q}{p} - \frac{q}{p}\frac{\lambda^2 \Delta t}{2},$$

where

$$q = \frac{2\lambda^2 \Delta t^2 - h^2}{12}, \qquad p = \Delta t - \frac{\lambda^2 h^2 \Delta t}{12} + \frac{\lambda^4 \Delta t^3}{12}.$$

The truncation error is therefore reduced to

$$E_{R_2} = e_5 \partial_x^5 u + e_6 \partial_x^6 u + \text{HOD}.$$

With the above constants, analysis of the conditions (D), (S), and (O) yields the following.

THEOREM 8. (i) *The* R2 *scheme satisfies conditions* (D) *if*

$$\alpha \leqslant \sqrt{6} \quad \text{and} \quad r \in [r_{d_2}, r_{d_1}] \qquad (56)$$
$$\alpha \geqslant \sqrt{6} \quad \text{and} \quad r \in [r_{d_1}, r_{d_2}],$$

where $r_{d_1} = \sqrt{3}/2\alpha^2$, $r_{d_2} = \sqrt{\alpha^2 - 3}/2\alpha^2$.

(ii) *The* R2 *scheme satisfies conditions* (S) *if*

$$\alpha \leqslant \sqrt{6} \quad \text{and} \quad r \in [r_{d_2}, r_{s_2}]$$
$$\sqrt{6} \leqslant \alpha \leqslant \frac{3\sqrt{3}}{2} \quad \text{and} \quad r \in [0, r_{s_3}] \cup [r_{d_2}, r_{s_2}] \tag{57}$$
$$\alpha \geqslant \frac{3\sqrt{3}}{2} \quad \text{and} \quad r \leqslant r_{d_2},$$

where

$$r_{s_{2,3}} = \left[\frac{2\alpha^2 - 9 \pm \sqrt{81 - 12\alpha^2}}{8\alpha^4}\right]^{1/2}.$$

(iii) *The* R2 *scheme satisfies condition* (O) *if*

$$\alpha \leqslant \sqrt{6} \quad \text{and} \quad r \in [r_{d_2}, r_0]$$
$$\alpha \geqslant \sqrt{6} \quad \text{and} \quad r \in [r_0, r_{d_2}], \tag{58}$$

with

$$r_0 = \frac{1}{2\alpha^2}\left[\frac{\alpha^3 - 3\alpha + 3}{1 + \alpha}\right]^{1/2}.$$

Proof. (i) Condition (D). $1 + A_1 + A_2 > 0$ yields the inequality

$$\frac{12 - 16\alpha^4 r^2}{12 - 4\alpha^2 + 16\alpha^4 r^2} > 0$$

and we easily deduce conditions (56).

(ii) Condition (S). $2r(A_1 - A_2) < 1$ yields the inequality

$$\frac{16\alpha^6 r^4 + r^2(36\alpha^2 - 8\alpha^4) + \alpha^2 - 6}{4\alpha^4 r^2 - \alpha^2 + 3} < 0 \tag{59}$$

and we must discuss the signs of both polynomials appearing in (59):

— the numerator has two positive roots,

$$r_{s_{2,3}} = \left[\frac{2\alpha^2 - 9 \pm \sqrt{81 - 12\alpha^2}}{8\alpha^4}\right]^{1/2}$$

when $\alpha < 3\sqrt{3}/2$ and no real roots when $\alpha > 3\sqrt{3}/2$,

— the denominator is positive when $\alpha < \sqrt{3}$ or when $\alpha \geqslant \sqrt{3}$ and $r > r_{d_2} = \sqrt{\alpha^2 - 3}/2\alpha^2$.

Therefore we conclude with the stability intervals (57).

(iii) Condition (O). $1 + A_1 + A_2 > \alpha$ yields the inequality

$$\frac{4\alpha^4(1+\alpha) r^2 - \alpha^3 + 3\alpha - 3}{4\alpha^4 r^2 - \alpha^2 + 3} < 0$$

with the same denominator as in (59). The numerator is positive if

$$r > r_0 = \frac{1}{2\alpha^2}\left[\frac{\alpha^3 - 3\alpha + 3}{1 + \alpha}\right]^{1/2}$$

and we deduce the non-oscillation intervals (58). ∎

In Fig. 5 we collect the results of Theorem 8 and observe the very limited range of useful values of r when α is about 2 or more; when $\alpha = \sqrt{6}$, the only acceptable value of r is $r = \sqrt{3}/12 \sim 0.144$, and for greater values of α, the useful interval of r is very sharp, e.g.,

$$\alpha = 3, \quad r \in [0.127, 0.136]$$
$$\alpha = 5, \quad r \in [0.087, 0.094].$$

The complexity of the expressions of A_i, B_i makes analysis of the positivity very difficult. Insofar as the useful interval of r is about 0.01 wide for values of α greater than 2, it does not appear important to consider the positivity of the scheme. We may only specify that the above domains (Fig. 5) are very slightly modified for positivity reasons.

Thus, the R2 scheme, which presents the best reduction of the discretization error, does not yield satisfactory numerical solutions (like schemes previously analyzed) for strongly convective problems.

R3 Scheme. The utilization of the R2 scheme is extremely sharp for strongly convective problems. Therefore, we relax one condition and consider the class of R3 schemes defined by

$$e_1 = e_2 = e_3 = 0 \tag{60}$$
$$E_{R_3} = O(\Delta t^2 + h^4); \tag{61}$$

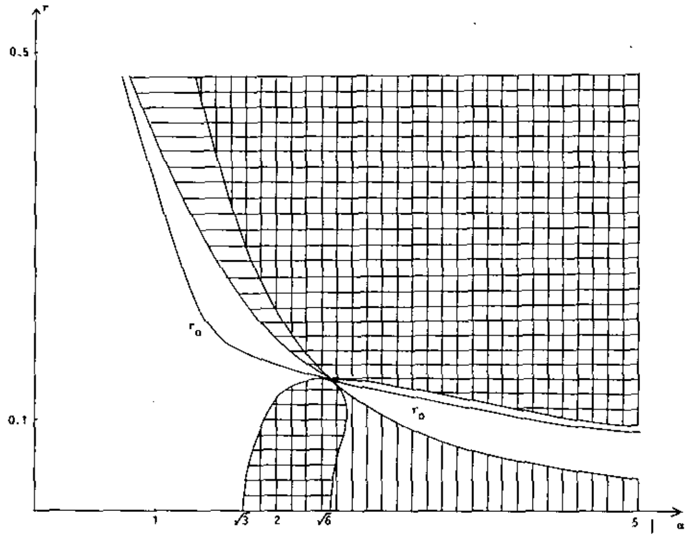

FIG. 5. The regions of the (α, r) plane in which the R2 scheme is unstable (horizontal shading) and does not satisfy condition (D) (vertical shading); r_0 is given by condition (O) (58).

i.e., A_i, B_i must be such that e_1, e_2, e_3, and the terms of order less than (2, 4) in e_4 vanish—the N and R2 schemes belong to this class.

As previously considered, we take $C=0$ and, prescribing (60) we express A_1, A_2, B_1 as a function of B_2:

$$\begin{aligned} B_1 &= -B_2 \\ A_2 &= -\frac{\lambda^2\,\Delta t}{12} - \frac{1}{6r} - B_2\left(1+\frac{\lambda^2\,\Delta t}{2}\right) \\ A_1 &= \frac{\lambda^2\,\Delta t}{12} + \frac{1}{6r} + B_2\left(1-\frac{\lambda^2\,\Delta t}{2}\right). \end{aligned} \tag{62}$$

Moreover, B_2 must be chosen so as to verify (61), i.e.,

$$e_4 = \frac{h^2}{12} - \frac{\lambda^2\,\Delta t^2}{6} + \frac{B_2}{12}\left[-\lambda^2 h^2\,\Delta t + 12\Delta t + \lambda^4\,\Delta t^3\right]$$

must be of order (2, 4).

In terms of B_2, conditions (D), (S), (O) become

$$\text{(D)} \qquad B_2 < \frac{1}{4\alpha^2 r} \tag{63}$$

$$\text{(S)} \qquad B_2 < \frac{1-4\alpha^2 r^2}{12r} \tag{64}$$

$$\text{(O)} \qquad B_2 < \frac{1-\alpha}{4\alpha^2 r}. \tag{65}$$

Remark. In the N scheme, $B_2 = -1/12r + \lambda^2\,\Delta t/12$ and, in the R2 scheme, B_2 is such that $e_4 = 0$. None of these choices corresponds to values of B_2 satisfying the three above inequalities (63)–(65).

The main objective is evidently to define B_2 so as to satisfy, if possible, conditions (63)–(65). We propose two possible choices for B_2; we examine the conditions (D), (S), and (O) and we consider the positivity of the schemes so defined.

R3A Scheme. The simplest choice for B_2 consists of

$$B_2 = -1/12r \tag{66}$$

which eliminates in e_4 the only terms depending on Δt and h^2. The coefficient of the leading term in the discretization error is then

$$e_4 = -\frac{\lambda^2\,\Delta t^2}{6} + \frac{\lambda^2 h^4}{144} - \frac{\lambda^4 h^2\,\Delta t^2}{144}.$$

For the above value of B_2, the inequalities (63)–(65) yield

Theorem 9. *The* R3A *scheme is stable if*

$$r \leqslant 1/\alpha\sqrt{2} \tag{67}$$

and satisfies the conditions (D) *and* (O) *for any value of* Δt, h.

Replacing B_2 in expressions (62) of A_1, A_2, we may write the coefficients of the difference scheme as

$$\begin{aligned} a_0 &= \frac{5}{6} + r - \frac{2\alpha^2 r^2}{3} + \frac{\alpha^2 r}{3} \\ a_1 &= \frac{1}{12} - \frac{r}{2} - \frac{\alpha}{12} + \frac{\alpha r}{2} - \frac{\alpha^2 r}{6} + \frac{\alpha^2 r^2}{3} \\ a_{-1} &= \frac{1}{12} - \frac{r}{2} + \frac{\alpha}{12} - \frac{\alpha r}{2} - \frac{\alpha^2 r}{6} + \frac{\alpha^2 r^2}{3} \\ b_0 &= \frac{5}{6} - r - \frac{2\alpha^2 r^2}{3} - \frac{\alpha^2 r}{3} \\ b_1 &= \frac{1}{12} + \frac{r}{2} + \frac{\alpha^2 r^2}{3} + \frac{\alpha^2 r}{6} - \frac{\alpha r}{2} - \frac{\alpha}{12} \\ b_{-1} &= \frac{1}{12} + \frac{r}{2} + \frac{\alpha^2 r^2}{3} + \frac{\alpha^2 r}{6} + \frac{\alpha r}{2} + \frac{\alpha}{12}. \end{aligned} \tag{68}$$

From the usual matrix formulation of the scheme

$$AV^{n+1} = BV^n,$$

we deduce

Theorem 10. (i) *B is a positive matrix if*

$$r < r_1 = \frac{\sqrt{\alpha^4 + 26\alpha^2 + 9} - (\alpha^2+3)}{4\alpha^2} \tag{69}$$

and, when $\alpha > 1$, *if*

$$r > r_2 = \frac{[\alpha^4 - 2\alpha^3 + 11\alpha^2 - 18\alpha + 9]^{1/2} - [\alpha^2 - 3\alpha + 3]}{4\alpha^2}. \tag{70}$$

(ii) *A is a DDL-matrix if the above conditions on B are satisfied.*

Proof. b_{-1} is always positive and the positivity of b_0, b_1 depends on the quadratic polynomial conditions,

$$4\alpha^2 r^2 + (2\alpha^2+6)r - 5 < 0$$

$$4\alpha^2 r^2 + (2\alpha^2 - 6\alpha + 6)r + 1 - \alpha > 0$$

which yield conditions (69)–(70) on r. If we write the quadratic inequalities corresponding to coefficients a_i, we observe that they yield conditions which are less restrictive than (69)–(70). ∎

We must remark that, if we compare r_2 and r_1, B is theoretically never positive when $\alpha > 3$ (but, the R3A scheme is, in practice, positive for precise values of r when $\alpha = 10$).

Figure 6 summarizes the results relative to the R3A scheme; the stability condition is not strongly restrictive and the practical limitations due to positivity allow the scheme to be utilized over a reasonable range of values of α (approximately [0; 4]). Thus, we observe appreciable progress, in comparison with the schemes previously analyzed. Finally, we attempt to propose an optimal scheme, considering a value of B_2 such that the three inequalities (63)–(65) are satisfied.

R3B SCHEME. The value of B_2 which defines this scheme is

$$B_2 = -\frac{1}{12r} - \frac{\lambda^2 \Delta t}{12} \qquad (71)$$

and from (62) we have

$$B_1 = -B_2, \qquad A_1 = +\frac{1}{12r} + \frac{\lambda^2 h^2}{24} + \frac{\lambda^4 \Delta t^2}{24},$$

$$A_2 = -\frac{1}{12r} + \frac{\lambda^2 h^2}{24} + \frac{\lambda^4 \Delta t^2}{24}.$$

THEOREM 11. *The R3B scheme defined above satisfies conditions (D), (S), and (O) for any value of Δt, h and the leading terms of its discretization error are given by*

$$E_{R_{3B}} = \left[\frac{\lambda^2 \Delta t^2}{4} - \frac{\lambda^2 h^4}{144}\right] \partial_x^4 u + \left[\frac{\lambda h^4}{80} - \frac{\lambda \Delta t^2}{4}\right] \partial_x^5 u + \left[\frac{\Delta t^2}{4} - \frac{h^2 \Delta t}{12} - \frac{h^4}{240}\right] \partial_x^6 u + \text{HOD}.$$

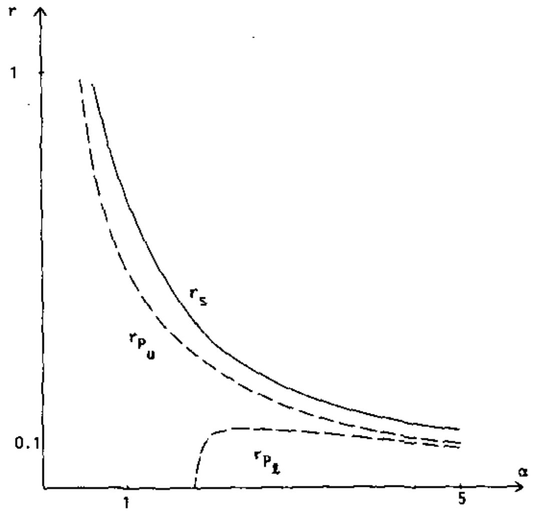

FIG. 6. R3A scheme: r_s stability limit given by (67); r_{P_l} and r_{P_u}, lower and upper experimental positivity limits.

This scheme satisfies the fundamental properties; we must examine the conditions of positivity based on the coefficients:

$$\begin{aligned}
b_0 &= \frac{5}{6} - \left(\frac{\alpha^2}{3} + 1\right) r - \frac{4\alpha^4}{3} r^3 \\
b_1 &= \frac{1}{12} - \frac{\alpha}{12} + \frac{r}{2} - \frac{\alpha r}{2} + \frac{\alpha^2 r}{6} - \frac{\alpha^3 r^2}{3} + \frac{2\alpha^4 r^3}{3} \\
b_{-1} &= \frac{1}{12} + \frac{\alpha}{12} + \frac{r}{2} + \frac{\alpha r}{2} + \frac{\alpha^2 r}{6} + \frac{\alpha^3 r^2}{3} + \frac{2\alpha^4 r^3}{3} \\
a_0 &= \frac{5}{6} + r + \frac{\alpha^2 r}{3} + \frac{4\alpha^4 r^3}{3} \\
a_1 &= \left(\frac{1}{12} - \frac{r}{2}\right)(1-\alpha) - \frac{\alpha^2 r}{6} - \frac{2\alpha^4 r^3}{3} - \frac{\alpha^3 r^2}{3} \\
a_{-1} &= \left(\frac{1}{12} - \frac{r}{2}\right)(1+\alpha) - \frac{\alpha^2 r}{6} - \frac{2\alpha^4 r^3}{3} + \frac{\alpha^3 r^2}{3}.
\end{aligned} \qquad (72)$$

This analysis, which requires a discussion about several cubic polynomials, does not yield analytical conditions on r and α. This drawback is not really crucial because:

(i) for given values of α, we may easily obtain computed conditions of positivity,

(ii) the study of the preceding FDS showed the significant differences between theoretical and effective conditions of positivity.

We give some partial results in the following proposition:

PROPOSITION. *If B is a positive matrix, the mesh ratio r satisfies*

$$\frac{\alpha - 1}{2\alpha^2} < r < \frac{\sqrt{9 + 24\alpha - 4\alpha^2} - 3}{4\alpha^2}. \qquad (73)$$

Proof. b_{-1} is always positive, the positivity of b_0 and b_1 corresponds to

$$8\alpha^4 r^3 + (2\alpha^2 + 6) r - 5 \leqslant 0 \qquad (74.1)$$

$$8\alpha^4 r^3 - 4\alpha^3 r^2 + 2r(\alpha^2 - 3\alpha + 3) + (1 - \alpha) \geqslant 0, \qquad (74.2)$$

which are simultaneously verified only if

$$4\alpha^3 r^2 + 6\alpha r + \alpha - 6 \leqslant 0; \tag{75}$$

(75) is valid if

$$r \leqslant \frac{\sqrt{9 + 24\alpha - 4\alpha^2} - 3}{4\alpha^2},$$

which is only possible if $\alpha < 6$.

Moreover, (74.2) is equivalent to

$$(1 - \alpha + 2\alpha^2 r)(1 + 6r + 4\alpha^2 r^2) > 16\alpha^2 r^2;$$

therefore, we must necessarily prescribe

$$1 - \alpha + 2\alpha^2 r > 0 \Leftrightarrow r > \frac{\alpha - 1}{2\alpha^2}.$$

Remarks. 1. From (74.1) we deduce a simple sufficient positivity condition for b_0,

$$r < r_p = \frac{5}{2\alpha^2 + 6}. \tag{76}$$

2. The study of the entries a_i (so that A is an DDL-matrix) does not provide constructive information.

In Fig. 7 we represent the necessary conditions (73), the sufficient condition (76), and the experimental positivity domain. We note that, even for relatively large values of α, the possible range of values is not too restricted. From this observation, combined with the properties of the scheme (Theorem 11), we may consider the R3B scheme as theoretically optimal among all the schemes previously analyzed.

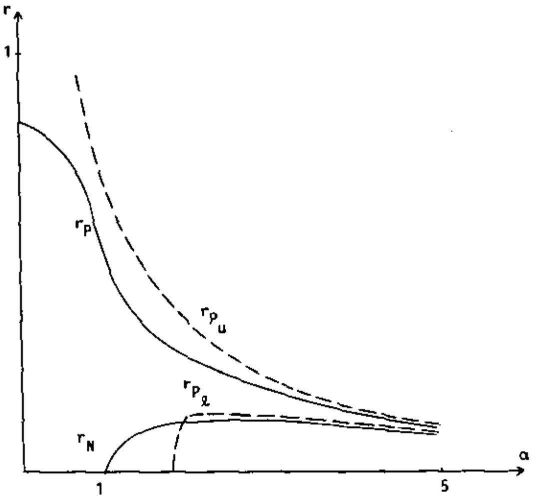

FIG. 7. R3B scheme: r_p positivity limit (76) (a sufficient condition); r_N: lower positivity limit (73) (a necessary condition); r_{P_l} and r_{P_u}, lower and upper experimental positivity limits.

5. NUMERICAL EXAMPLES

All the schemes analyzed in the preceding sections are formally of order (2, 4). Until now, we have neglected the effective accuracy of the computed numerical solutions. So we propose some numerical tests so as to compare the behaviour of solutions produced by the different fourth-order schemes in reference to the solutions obtained with the most efficient second-order schemes [1].

We first consider the advection–diffusion of a Gaussian pulse centred at $x = 0.2$,

$$u_0(x) = \exp[-[x - 0.2]^2]. \tag{77}$$

The solution of ($\mathscr{P}$) on $[0, 1] \times [0, T[$ is given by

$$u(x, t) = g(x, t) = \frac{1}{\sqrt{4t+1}} \exp\left[-\frac{(x - 0.2 - \lambda t)^2}{4t + 1}\right], \tag{78}$$

provided that the boundary conditions are coherent with (78), i.e.,

$$u(0, t) = g(0, t)$$
$$u(1, t) = g(1, t).$$

This example amply satisfies regularity hypotheses and therefore allows precise tests to be made on the discretization error. Noye utilized this problem in [7] and like him we consider a time interval $[0, T]$, such that the pulse is centred at $x = 0.8$ at time T. We must remark that these tests require a few time steps and do not exactly reflect the asymptotic properties of the schemes (stability, oscillation) —some numerical results in Table I are obtained with moderately unstable schemes.

For a wide range of values of α, Table I gives the maximum absolute error,

$$\varepsilon = \max_j |v_j^N - u(x_j, T)|,$$

produced by each fourth-order scheme, in comparison with three efficient second-order schemes:

(i) The WZ scheme, a three-level weighted scheme due to Zlamal [2, 16, 17],

$$(\theta + \tfrac{1}{2})\, v_j^{n+1} - 2\theta v_j^n + (\theta - \tfrac{1}{2})\, v_j^{n-1} = \Delta t\, A_h[\beta v_j^{n+1} + (1 + \theta - 2\beta)\, v_j^n + (\beta - \theta)\, v_j^{n-1}] \tag{79}$$

with $\beta = (1 + \theta)^2/4$ and $A_h = D_+ D_- - \lambda D_0$;

TABLE I

Cell Reynolds number α		0.2	0.5	1.5	2.5	4	10
Time interval T		0.075	0.03	0.01	0.006	0.00375	0.0015
M1 scheme	r	2	1.2	0.5	Unstable	0.1	0.04
	ε	0.171 (−3)	0.398 (−3)	0.682 (−3)		0.287 (−2)	0.461 (−3)
M2 scheme	r	2	1.2	0.5	0.2	0.1	0.04
	ε	0.171 (−3)	0.393 (−3)	0.669 (−3)	0.301 (−3)	0.198 (−3)	0.261 (−3)
W scheme	r	2	1.2	0.5	0.2	Unstable	Unstable
	ε	0.168 (−3)	0.377 (−3)	0.468 (−3)	0.294 (−3)		
N scheme	r	2	1.2	0.3	0.2	0.1	0.04
	ε	0.470 (−4)	0.812 (−4)	0.258 (−4)	0.191 (−4)	0.715 (−6)	0.147 (−4)
R1 scheme	r	2	1.2	0.5	0.2	0.1	0.04
	ε	0.149 (−3)	0.278 (−3)	0.317 (−3)	0.637 (−4)	0.410 (−4)	0.165 (−3)
R2 scheme	r	2	1.2	0.25	0.14	0.1	0.04
	ε	0.270 (−4)	0.802 (−4)	0.173 (−5)	0.536 (−6)	0.834 (−6)	0.477 (−6)
R3A scheme	r	2	1.2	0.5	0.2	0.1	0.04
	ε	0.101 (−3)	0.162 (−3)	0.122 (−3)	0.287 (−4)	0.554 (−5)	0.403 (−4)
R3B scheme	r	2	1.2	0.5	0.2	0.1	0.04
	ε	0.155 (−3)	0.240 (−3)	0.214 (−3)	0.411 (−4)	0.966 (−5)	0.557 (−4)
WZ scheme	r	2	1.2	0.5	0.2	0.1	0.04
	ε	0.459 (−3)	0.936 (−3)	0.145 (−2)	0.102 (−2)	0.107 (−2)	0.130 (−2)
MFTCS scheme	r	0.4	0.4	0.25	0.15	0.1	0.04
	ε	0.370 (−3)	0.648 (−3)	0.561 (−3)	0.263 (−3)	0.142 (−3)	0.693 (−4)
Samarskii scheme	r	0.4	0.4	0.25	0.15	0.1	0.04
	ε	0.449 (−3)	0.168 (−2)	0.436 (−2)	0.112 (−2)	0.142 (−3)	0.323 (−2)

(ii) The MFTCS scheme [1, 7, 13, 18] which uses a Lax–Wendroff correction of the artificial viscosity,

$$v_j^{n+1}=\left[1+\Delta t\left[\left(1+\lambda^2\frac{\Delta t}{2}\right)D_+D_- -\lambda D_0\right]\right]v_j^n; \quad (80)$$

(iii) the Samarskii [1, 19] explicit scheme, an upstream scheme with correction of the artificial viscosity,

$$v_j^{n+1}=[1+\Delta t[(1+\alpha)^{-1}D_+D_- -\lambda D_-]]\,v_j^n. \quad (81)$$

These schemes are of order (2, 2) (WZ scheme) and (1, 2) (MFTCS and Samarskii schemes).

The numerical experiments used a fixed space step $h=0.05$ for different values of the convection velocity λ: $\lambda=8$, 20, 60, 100, 160, 400, which correspond to the following values of the cell Reynolds number α: $\alpha=0.2$, 0.5, 1.5, 2.5, 4, 10.

For a valid comparison of the accuracy of the FDS, we utilized the same mesh ratio r as much as possible in the intervals defined in Sections 3 and 4. Table I completes the main results given in the previous sections and agrees with the discretization errors relative to each scheme:

— the R2 scheme is by far the most accurate,

— the R3 schemes give very satisfactory results,

— the other schemes which retain more components in the truncation error are less accurate.

We must recall that the working area of the R2 scheme is very sharp when α is relatively large (the MFTCS scheme which yields good numerical results presents the same behaviour [1]).

The propagation of the Gaussian pulse from $x=0.2$ ($t=0$) to $x=0.8$ ($t=T$) is well reproduced by fourth-order schemes: the relative error on the peak height is about 2×10^{-4} for all the schemes in Table I, except for the Samarskii scheme which presents a 0.3% error (for infor-

TABLE II

		R3 scheme	WZ scheme	MFTCS scheme
$h=0.1$, $\alpha=0.8$	ε_2	0.1907 (−2)	0.1457 (−1)	0.4200 (−2)
$h=0.05$	ρ_1	12.58	5.77	3.42
$\alpha=0.4$	ε_2	0.1515 (−3)	0.2523 (−2)	0.1228 (−2)
$h=0.025$	ρ_2	21.86	3.77	2.98
$\alpha=0.2$	ε_2	0.6933 (−5)	0.6691 (−3)	0.4122 (−3)
$h=0.1$, $\alpha=10$	ε_2	0.2016 (−3)	0.1100 (−1)	0.7461 (−3)
$h=0.05$	ρ_1	8.65	3.81	1.92
$\alpha=5$	ε_2	0.2331 (−4)	0.2884 (−2)	0.3887 (−3)
$h=0.025$	ρ_2	5.63	3.11	2.92
$\alpha=2.5$	ε_2	0.4144 (−5)	0.9286 (−3)	0.1333 (−3)

mation, this error is about +2% for the explicit centred scheme and −2% for the basic upstream scheme).

Insofar as we consider moderate or large values of α, the effective order of the discretization error is dependent on the range of values of α. In Table II we illustrate the error decrease for three schemes:

- the WZ scheme of order (2, 2)
- the MFTCS scheme of order (1, 2)
- an R3 scheme of order (2, 4).

We consider two situations:

- $\lambda = 16$, $h = 0.1, 0.05, 0.025$, i.e., $\alpha = 0.8, 0.4, 0.2$;
- $\lambda = 200$, $h = 0.1, 0.05, 0.025$, i.e., $\alpha = 10, 5, 2.5$.

We report the l_2 errors,

$$\varepsilon_2 = \left[\sum_j |v_j^N - u(x_j, T)|^2\right]^{1/2},$$

and the decrease factors,

$$\rho_1 = \frac{\varepsilon_2(h)}{\varepsilon_2(h/2)}, \qquad \rho_2 = \frac{\varepsilon_2(h/2)}{\varepsilon_2(h/4)}.$$

We observe that the error decreases roughly agree with the order of the schemes when $\alpha < 1$. On the other hand, the effective order of the schemes is significantly lower than the theoretical order when $\alpha > 1$; the order of the R3 scheme is hardly over 2 and that of the MFTCS scheme is about 1.

For completeness, we carried out some numerical experiments with the following discontinuous data:

(i) initial condition $u(x, 0) = 1$ in $]0, 1]$

(ii) boundary conditions $u(0, t) = 0$ and $u(1, t) = 1$ for t in $[0, T[$.

A formal analytical solution of ($\mathscr{P}$) with these data may be obtained but it does not provide readily available results for large values of λ. Thus, the comparisons were made with an "exact" solution obtained with a very fine mesh (e.g., $h = 0.002$).

In comparison with the previous example, the accuracy of the numerical results is significantly restricted, in particular, for large values of α. The absence of smoothness of the data notably reduces the effective convergence order of the schemes and, consequently, the fourth-order schemes, which require the existence of higher order derivatives, become hardly more accurate than second-order schemes (the pointwise error is approximately reduced by a factor two).

These experiments outline the characteristics of the different properties analyzed in Sections 3 and 4:

— if conditions (D) are not satisfied, the FDS cannot yield acceptable numerical solutions;

— if conditions (S) and/or (O) are not satisfied, we may frequently obtain numerical solutions during a few time steps but the implementation of FDS over a rather large time interval gives

- unbounded numerical solutions (instability)
- strongly oscillatory solutions (if condition (O) is not verified).

On the other hand, the non-positivity of an FDS, which is inconsistent with the differential problem ($\mathscr{P}$), does not exclude the obtaining of satisfactory numerical results.

Figures 8–10 summarize these observations and outline that the choice of a difference scheme for strongly convective problems requires careful investigation:

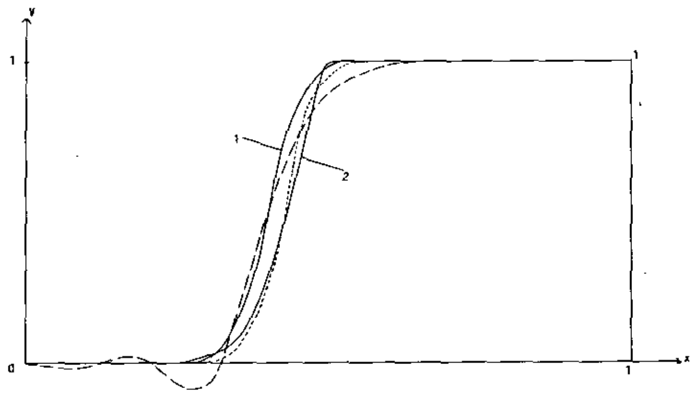

FIG. 8. Exact profile (1) and approximate profiles given by the Samarskii (2), R3B (dotted line) and M2 (broken line) schemes for $\lambda = 400$, $t = 0.001$.

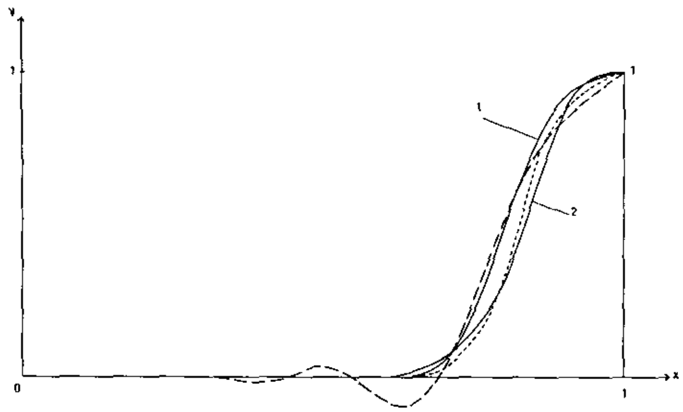

FIG. 9. Exact profile (1) and approximate profiles given by the Samarskii (2), R3B (dotted line) and M2 (broken line) schemes for $\lambda = 400$, $t = 0.002$.

— properties analyzed in Sections 3 and 4,

— characteristics of ($\mathscr{P}$); smoothness of the solutions, research of transient-state solutions, or quasi-steady-state solutions, etc.

We plotted the numerical solutions obtained with three representative schemes: M2, R3B, and Samarskii schemes, for $\alpha = 10$ over a time interval $[0; 0.006]$; for a large convection velocity ($\lambda = 400$), this interval allows steady-state solutions to be approached.

The M2 scheme yields oscillatory numerical solutions:

1. during the transient state because the scheme is not positive;

2. when approaching the steady-state solutions because condition (O) is not satisfied.

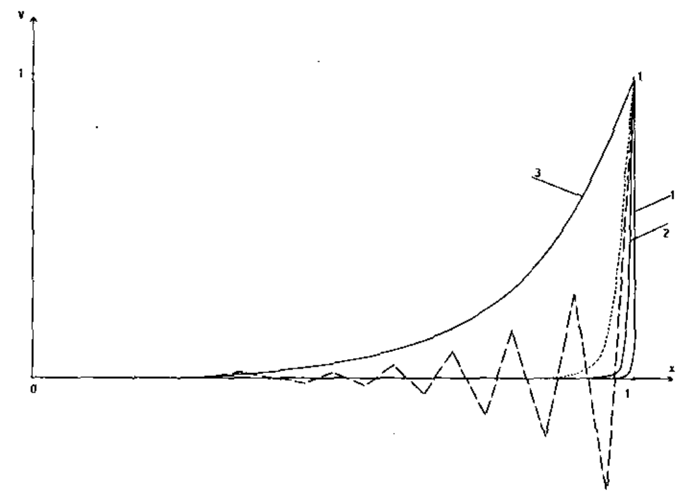

FIG. 10. Exact profile (1) and approximate profiles given by the Samarskii (2), R3B (3) with $C = 0$, R3B (dotted line) with $C = 60$, and M2 (broken line) schemes for $\lambda = 400$, $t = 0.006$.

It should be noted that in (1) the steep velocity profile is correctly approximated: the pointwise error is about 10^{-1} (as opposed to 2×10^{-1} for many other schemes). The oscillatory behaviour of the scheme progressively destroys the numerical solutions (situation 2)).

The R3B scheme (like the R3A, R2, and N schemes) yields acceptable transient-state numerical solutions if the step ratio r is conveniently chosen (this choice is extremely sharp for the R2 scheme). As specified in the preliminary remark of Section 4, the choice of constant C becomes crucial if one wants to compute virtually steady-state solutions. The solution obtained for $t = 0.006$ presents a great amount of numerical diffusion when $C = 0$ and we also give in Fig. 10 the numerical solution computed with $C \sim A_1 + A_2$ ($C = 60$ in this example); the influence of C is very limited during the transient state and extremely important in steady-state solutions.

It is perhaps necessary to outline that the absence of oscillations does not absolutely guarantee the accuracy of the numerical solutions.

The Samarskii second-order explicit scheme is not very accurate but it works conveniently during the time scale considered in this example; the propagation of the velocity profile ($t = 0.001$ and 0.002) and the boundary layer ($t = 0.006$) are correctly approximated.

This numerical test corresponds to quite a difficult situation: discontinuous data and large cell Reynolds number. On the basis of the theoretical results given in Sections 3 and 4, we may obtain accurate numerical solutions for lower values of α.

6. CONCLUSION

We produced an extensive analysis of several fourth-order schemes in a general framework, incorporating some schemes already proposed by different authors [6–8]. We assigned to these schemes the basic conditions necessary to obtain numerical solutions; i.e., we only considered

— non-anti-diffusive schemes $\leftrightarrow$ conditions (D)

— stable schemes $\leftrightarrow$ conditions (S)

— non-oscillatory schemes $\leftrightarrow$ condition (O).

Moreover, we analyzed the positivity of all the FDS. These schemes being generally non-commutative, we only obtained sufficient (but frequently too restrictive) conditions which need to be completed by numerical tests of the positivity. This evaluation gives conditions under which an FDS (which satisfies conditions (D), (S), and (O)) yields satisfactory numerical results.

The results and the discussion essentially focus on the cell Reynolds number α, because our main objective is to obtain efficient numerical solutions for strongly convective problems.

The main conclusions of this work are the following:

(1) The fourth-order schemes are very suitable for differential problems where the diffusion phenomenon is not negligible, i.e., yielding discrete problems where α is less than or hardly over unity.

(2) The properties of the FDS may differ greatly (even for schemes which are constructed in the same way, e.g., schemes M1 and M2), thus a careful study of each FDS is necessary.

(3) Although they are implicit, these FDSs always present an acceptable maximum mesh ratio (when α is relatively large) when one of the basic properties is lacking. This maximum mesh ratio behaves like α^{-1}. Obviously, the reason which yields the leading restriction on r is important; a stability limit is an effective barrier, whereas positivity conditions are much less restraining and depend slightly on the data of the differential problem.

(4) Theoretical analysis states that the N scheme (among schemes already proposed) and the R3 schemes (proposed in the present paper) offer the best compromise and are efficient for values of $\alpha \simeq 5$.

(5) For strongly convective problems ($\lambda \gg 1$), theoretical results and numerical experiments must be exhaustively examined; the actual order of accuracy is less than 4 and different kinds of oscillation may spoil the results.

In this case, some explicit second-order schemes (e.g., MFTCS and Samarskii schemes thoroughly analyzed in [1]) *may yield numerical results that are almost as satisfactory* (and less costly).

Beyond the specific items, one important point must be mentioned. All these FDS may be written for variable coefficient differential problems (e.g., M1 and M2 schemes in [6]) but such a formulation would considerably lengthen the paper. The basic properties are clearly valid for the associated frozen coefficient problems and may be generalized for sufficiently smooth coefficients. The main difficulty is the extension of stability properties. Kreiss [20] gave the conditions which must be satisfied by $(\mathscr{P})$ and (P_h) for the transition from frozen coefficient problems to variable coefficient problems.

Briefly, if the coefficients are sufficiently smooth, the properties of the FDS will be maintained (the quantitative results will be obviously less precise). On the other hand, if we consider quasilinear problems (λ is replaced by the unknown function u), these fourth-order schemes present important algorithmic (and also theoretical) difficulties; at every time step, we have to solve a non-linear system, and, if we linearize it, the order of accuracy is then less than 4. *Thus, these schemes are not suitable for quasi-linear* prolems and a better approach is to consider specific explicit *second-order schemes (see 5°) in this section).*

The next objective is the analysis of fourth-order schemes for multidimensional problems. Some 2D or 3D fourth-order schemes have been proposed [6, 21, e.g.]; the nine-point fourth-order schemes applied to 2D elliptic problems are well known and must support fourth-order schemes associated with $(\mathscr{P})$.

Except for schemes which are factorized into 1D schemes, the analysis of the properties of the FDS presents important technical difficulties (see Rigal [22] for a nine-point second-order scheme). Although a general approach (extension of this paper) does not seem to be feasable as yet, we are currently considering an exhaustive analysis of some 2D schemes.

REFERENCES

1. A. Rigal, *Int. J. Numer. Methods Engng.* **28**, 1001 (1989).
2. A. Rigal, *Int. J. Numer. Methods Engng.* **30**, 307 (1990).
3. M. Ciment, S. H. Leventhal, and B. C. Weinberg, *J. Comput. Phys.* **28**, 135 (1978).
4. S. C. R. Dennis and J. D. Hudson, *J. Comput. Phys.* **85**, 390 (1989).
5. S. R. K. Iyengar and R. C. Mittal, *J. Inst. Math. Appl.* **22**, 321 (1978).
6. R. Manohar, S. R. K. Iyengar, and U. A. Krishnaiah, *J. Comput. Phys.* **77**, 513 (1988).
7. B. J. Noye, *Commun. Appl. Numer. Methods* **6**, 279 (1990).
8. R. D. Richtmyer and K. W. Morton, *Difference Methods for Initial Value Problems* (Wiley, New York, 1967).
9. R. F. Warming and B. J. Hyett, *J. Comput. Phys.* **14**, 159 (1974).
10. S.-C. Chang, *J. Comput. Phys.* **86**, 107 (1990).
11. B. J. Noye and H. H. Tan, *Int. J. Numer. Methods Fluids* **9**, 75 (1989).
12. D. F. Griffiths and J. M. Sanz-Serna, *SIAM J. Sci. Stat. Comput.* **7**, 994 (1986).
13. A. C. Hindmarsh, M. M. Gresho, and D. F. Griffiths, *Int. J. Numer. Methods Fluids* **4**, 853 (1984).
14. K. W. Morton, *Int. J. Numer. Methods Engng.* **15**, 677 (1980).
15. C. Bolley and M. Crouzeix, *RAIRO Anal. Numér.* **12**, 237 (1978).
16. J. M. Varah, *SIAM J. Numer. Anal.* **17**, 300 (1980).
17. M. Zlamal, in *The Mathematics of Finite Elements and Applications II, Brunel University, United Kingdom, 1975*, edited by J. R. Whiteman (Academic Press, London, 1976), p. 85.
18. J. L. Siemeniuch and I. Gladwell, *Int. J. Numer. Methods Engng.* **11**, 1667 (1977).
19. M. M. Gupta, *Int. J. Numer. Methods Fluids* **3**, 339 (1983).
20. H. O. Kreiss, *Séminaire de Mathématiques Supérieures* (Université de Montréal, Montréal, 1978).
21. M. K. Jain, R. K. Jain, and R. K. Mohanty, *Int. J. Comput. Math.* **38**, 101 (1991).
22. A. Rigal, *Int. J. Numer. Methods Fluids* **13**, 579 (1991).