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ANALYSIS AND EXPERIMENTS OF A SET OF THREE-LEVEL SEMI-IMPLICIT FINITE DIFFERENCE SCHEMES FOR NONLINEAR PARABOLIC EQUATIONS

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Abstract

We investigate a number of three-level (two step) finite difference schemes for time discretization in solving a class of nonlinear parabolic partial differential equations (PDE's). In contrast with two-level (one step) implicit schemes, where a nonlinear system of algebraic equations has to be solved, our proposed schemes are semi-implicit (or linearly implicit). Therefore the implementation is simple since only the solution of a linear system is needed at each time step. Linear stability analysis together with local truncation error estimates are provided for all schemes considered. We finally illustrate the schemes by applying them to one linear and four nonlinear parabolic equations. Test results show that the stability of these numerical schemes is well predicted by the linear theory.

AMS (MOS) Subject Classifications : 65M10, 39A11, 35K15.

Key words : Nonlinear Parabolic PDE's, Three-Level Schemes, Stability, Linearization.

Running Head : Three-Level Finite Difference Schemes.

Contents

1 Introduction

In this report we shall consider the finite difference solution of the nonlinear parabolic partial differential equations (PDE's)

$$\frac{\partial f}{\partial t} = D(f)\frac{\partial^2 f}{\partial x^2} + C(f, \frac{\partial f}{\partial x}) \tag{1}$$

in the region $0 \leq x \leq 1,\ t \geq 0$, where $f(x,0)$, $f(0,t)$ and $f(1,t)$ are prescribed. Assume that in (1), both $D(f)$ and $C(f, f_x)$ are nonlinear but smooth functions. Of course we require equation (1) to have an unique solution F. For the stability analysis we shall replace (1) by a linear model equation

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2} + Dk\frac{\partial f}{\partial x} \tag{2}$$

where $D,\ k$ are taken to be constants with $D > 0$. The choice of C is based on similarity to semiconductor models.

Let us adopt the usual notation for stepsizes Δx in space and Δt in time. Denote the finite difference solution by $f(n\Delta x, j\Delta t) = f_n^j$. For brevity we shall denote the central differences by

$$\begin{aligned} \delta f_n^j &= f_{n+1}^j - f_{n-1}^j && \text{first order} \\ \delta^2 f_n^j &= f_{n+1}^j - 2f_n^j + f_{n-1}^j && \text{second order} \end{aligned}$$

The idea of using three time level schemes, instead of two say, is to theoretically increase the accuracy and stability, and to be able to practically linearize the nonlinear algebraic systems which are usually generated from using implicit schemes and difficult or expensive to solve. Our proposed three-level schemes will all be of the form

$$\frac{1}{\Delta t}\sum_{\ell=0}^{2} w_\ell f_n^{j+\ell} = \frac{D(f_n^{j+1})}{\Delta x^2}\sum_{\ell=0}^{2}\sum_{m=-1}^{1} \bar{w}_\ell^{(m)} f_{n+m}^{j+\ell} + C\left(\sum_{\ell=0}^{2} \tilde{w}_\ell f_n^{j+\ell}, \frac{1}{\Delta x}\sum_{\ell=0}^{2} \hat{w}_\ell f_n^{j+\ell}\right), \tag{3}$$

where w_ℓ, $\bar{w}_\ell^{(m)}$, $\tilde{w}_\ell$ and $\hat{w}_\ell$ are appropriate constants. Refer to Fig.1 for the molecular stencil of (3), where j refers to the known level, $j+1$ the intermediate level and $j+2$ the new time level. Note that in (3) the coefficient function D is always evaluated at the intermediate level. As we shall discuss later, some terms of the function C will be linearized if $\tilde{w}_2$ or $\hat{w}_2$ are not zero.

Therefore the nonlinear PDE (1) is to be approximately solved through the 'linearized' finite difference equation (3). Specific schemes to be studied here are all of the general form (3) and hence can be easily implemented, as the resulting linear system has at most a tridiagonal coefficient matrix.

In section 2 we shall introduce the first five schemes, all based on the idea of the 'leap-frog' scheme. These have been generalized from the two-level schemes tabulated in Richtmyer and Morton [8, Ch.8] to solve equation (1). In section 3 we consider the three-level fully explicit scheme of Du Fort and Frankel [2] for our problem. In section 4 the Varah [12] scheme, proposed for mildly nonlinear equations, is generalized for solving the nonlinear equation (1). Local error analysis of all schemes are given in section 5. Finally in section 6 we carry out numerical experiments for five test examples and in section 7 we draw our conclusions.

2 Semi-implicit three-level schemes

Scheme 1 (backward Euler time stepping)

$$\frac{f_n^{j+2} - f_n^j}{2\Delta t} = \frac{D(f_n^{j+1})}{\Delta x^2}\delta^2 f_n^{j+2} + C(f_n^{j+1}, \frac{\delta f_n^{j+1}}{2\Delta x}) \tag{4}$$

For the linear model equation (2), we have

$$(1 - \sigma\delta^2) f_n^{j+2} = \omega\delta f_n^{j+1} + f_n^j \tag{5}$$

where $\sigma = 2D\Delta t/\Delta x^2$ and $\omega = Dk\Delta t/\Delta x$. The stability of Scheme 1 follows from

THEOREM 1 *Scheme 1 for equation (2), i.e. (5), is A-stable if*

$$\Delta t < \frac{\Delta x}{D|k|}.$$

Proof. Write equation (5) in an equivalent form

$$\begin{pmatrix} 1 - \sigma\delta^2 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} f_n^{j+2} \\ g_n^{j+2} \end{pmatrix} = \begin{pmatrix} \omega\delta & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} f_n^{j+1} \\ g_n^{j+1} \end{pmatrix}$$

following Richtmyer and Morton [8, Ch.7]. Then the amplification matrix (associated with the β component of Fourier variable) is given by

$$G(\xi, \Delta t) = \begin{pmatrix} \frac{bi}{1+a} & \frac{1}{1+a} \\ 1 & 0 \end{pmatrix}$$

where $\xi = \beta\Delta x$, $a = 4\sigma \sin^2\frac{\xi}{2}$ and $b = 2\omega \sin \xi$ (since $\delta(e^{i\beta x_n}) = 2i \sin \xi \; e^{i\beta x_n}$ and $\delta^2(e^{i\beta x_n}) = -4\sin^2\frac{\xi}{2} \; e^{i\beta x_n}$). The eigenvalues μ of the matrix G satisfy

$$(1+a)\mu^2 - bi\mu - 1 = 0. \tag{6}$$

From the Appendix, we know that the roots of (6) satisfy $|\mu| < 1$ if and only if (the Schur criterion)

$$1) \quad d_1 = (1+a)^2 - 1 = a^2 + 2a > 0;$$

$$2) \quad d_2 = |bi - (1+a)bi| = a|b| < d_1.$$

Obviously the first inequality is true except when $\xi = 0$. Since $a \geq 0$, the second inequality requires that $|b| < a+2$ or $|b| < 2$. That is, $|2\omega \sin \xi| < 2$. Thus a sufficient condition is $|Dk\Delta t/\Delta x| < 1$ *i.e.* $\Delta t < \Delta x/(D|k|)$. □

Scheme 2 (Richtmyer and Morton [8, p.190], No.9)

$$\frac{3}{2}\frac{f_n^{j+2} - f_n^{j+1}}{\Delta t} - \frac{1}{2}\frac{f_n^{j+1} - f_n^j}{\Delta t} = \frac{D(f_n^{j+1})}{\Delta x^2}\delta^2 f_n^{j+2} + C(f_n^{j+1}, \frac{\delta f_n^{j+1}}{2\Delta x}) \tag{7}$$

For the linear model equation (2), we obtain

$$(3 - \sigma\delta^2) f_n^{j+2} = (4 + \omega\delta) f_n^{j+1} - f_n^j \tag{8}$$

with $\sigma = 2D\Delta t/\Delta x^2$ and $\omega = Dk\Delta t/\Delta x$.

<u>**THEOREM**</u> **2** *Scheme 2 for equation (2), i.e. (8), is A-stable if*

$$\Delta t < \frac{1}{Dk^2}.$$

<u>Proof</u>. Denote again $a = 4\sigma \sin^2 \frac{\xi}{2}$ and $b = 2\omega \sin \xi$. Then the amplification matrix is given by

$$\begin{pmatrix} \frac{4+bi}{3+a} & -\frac{1}{3+a} \\ 1 & 0 \end{pmatrix},$$

with the eigenvalues μ satisfying

$$(3 + a)\mu^2 - (4 + bi)\mu + 1 = 0. \tag{9}$$

For $|\mu| < 1$, we require by the Schur criterion (see Appendix)

1) $d_1 = (3 + a)^2 - 1 = (a + 4)(a + 2) > 0;$

2) $d_2 = |-4 - bi - (3 + a)(-4 + bi)| = \sqrt{4^2(2 + a)^2 + b^2(4 + a)^2} < d_1.$

The first inequality is always true. The second inequality may be written as

$$\frac{4^2}{(4+a)^2} + \frac{b^2}{(2+a)^2} < 1,$$

i.e.

$$\frac{b^2}{a} < \left(\frac{a+2}{a+4}\right)^2 (a+8). \qquad (10)$$

Now the left hand side of (10), after substitution of b and a, becomes

$$4\left(\frac{Dk\Delta t}{\Delta x}\right)^2 \sin^2\xi \Big/ \left(4\frac{2D\Delta t}{\Delta x^2}\sin^2\frac{\xi}{2}\right) = 2Dk^2\Delta t\cos^2\frac{\xi}{2} \leq 2Dk^2\Delta t.$$

On the other hand, the right hand side of (10) is bounded from below by

$$\left(\frac{a+2}{2a+4}\right)^2 (a+8) = \frac{8+a}{4} \geq 2.$$

Thus we are able to satisfy the inequality (10) from the sufficient condition $2Dk^2\Delta t < 2$ *i.e.* $\Delta t < \frac{1}{Dk^2}$. $\square$

Scheme 3 (Mitchell and Griffiths [7, p.99])

$$\frac{f_n^{j+2} - f_n^j}{2\Delta t} = \frac{D(f_n^{j+1})}{\Delta x^2}\delta^2\left(\frac{f_n^{j+2} + f_n^{j+1} + f_n^j}{3}\right) + C(f_n^{j+1}, \frac{\delta f_n^{j+1}}{2\Delta x}) \qquad (11)$$

Applying (11) to the linear model equation (2), we obtain

$$(3-\sigma\delta^2)f_n^{j+2} = (\sigma\delta^2 + 3\omega\delta)f_n^{j+1} + (3+\sigma\delta^2)f_n^j \qquad (12)$$

where $\sigma = 2D\Delta t/\Delta x^2$ and $\omega = Dk\Delta t/\Delta x$.

THEOREM 3 *Scheme 3 for equation (2), i.e. (12), is A-stable if*

$$\Delta t < \frac{\sqrt{3}\Delta x}{2D|k|}.$$

Proof. The amplification matrix is given by

$$\begin{pmatrix} \frac{3bi-a}{3+a} & \frac{3-a}{3+a} \\ 1 & 0 \end{pmatrix},$$

with the eigenvalues μ satisfying

$$(3+a)\mu^2 + (a-3bi)\mu + (a-3) = 0, \qquad (13)$$

where as before $a = 4\sigma\sin^2\frac{\xi}{2}$ and $b = 2\omega\sin\xi$. Using the Schur criterion, we require for $|\mu| < 1$

1) $d_1 = (a+3)^2 - (a-3)^2 = 12a > 0;$

2) $d_2 = |(a-3)(a-3bi) - (a+3)(a+3bi)| = 6a\sqrt{1+b^2} < d_1.$

The first inequality is true except when $\xi = 0$. The second inequality simply becomes $|b| <$

$\sqrt{3}$, *i.e.* $|b| = 2\frac{|k|D\Delta t}{\Delta x}|\sin\xi| < \sqrt{3}$. Then a sufficient condition is $\Delta t < \sqrt{3}\Delta x/(2D|k|)$. □

Note that in Varah [12] the condition $\Delta t < \Delta x/(D|k|)$ is given. For diffusion dominated problems, this scheme is known to lead to improper decay in numerical solutions (refer to Varah [12] and Cash [1]). The scheme 3, which is second order in both space and time (see §5), was first proposed by Lees [3].

Scheme 4 (Crank-Nicolson type, Svoboda [11, Ch.4])

$$\frac{f_n^{j+2} - f_n^j}{2\Delta t} = \frac{D(f_n^{j+1})}{\Delta x^2}\delta^2\left(\frac{f_n^{j+2} + f_n^j}{2}\right) + C(f_n^{j+1}, \frac{\delta f_n^{j+1}}{2\Delta x}) \tag{14}$$

Applying (14) to the linear model equation (2) gives rise to

$$(1 - \sigma\delta^2)f_n^{j+2} = \omega\delta f_n^{j+1} + (1 + \sigma\delta^2)f_n^j \tag{15}$$

where $\sigma = D\Delta t/\Delta x^2$ and $\omega = Dk\Delta t/\Delta x$.

THEOREM 4 *Scheme 4 for equation (2), i.e. (15), is A-stable if*

$$\Delta t < \frac{\Delta x}{D|k|}.$$

Proof. For (15), we write its amplification matrix as

$$\begin{pmatrix} \frac{bi}{1+a} & \frac{1-a}{1+a} \\ 1 & 0 \end{pmatrix},$$

whose eigenvalues μ satisfy

$$(a+1)\mu^2 - bi\mu + (a-1) = 0, \tag{16}$$

where as before $a = 4\sigma \sin^2 \frac{\xi}{2}$ and $b = 2\omega \sin \xi$. The Schur criterion requires for $|\mu| < 1$

$$1) \quad d_1 = (a+1)^2 - (a-1)^2 = 4a > 0;$$

$$2) \quad d_2 = |(a-1)(-bi) - (a+1)(bi)| = 2a|b| < d_1.$$

The first inequality is satisfied except when $\xi = 0$. The second inequality gives $|b| < 2$, *i.e.* $\Delta t |\sin \xi| < \Delta x/(D|k|)$. Hence the sufficient condition is $\Delta t < \Delta x/(D|k|)$. □

Remark : If the averaging in (14) occurs between levels $j+2$ and $j+1$, then the resulting scheme may be named as 4a. For the linear model (2), the scheme 4a is always unstable. This can be shown as follows. For the new scheme 4a, corresponding to (15) of Scheme 4, we have

$$(1 - \sigma\delta^2) f_n^{j+2} = (\sigma\delta^2 + \omega\delta) f_n^{j+1} + f_n^j \tag{17}$$

and then the new amplification matrix is

$$G(\xi, \Delta t) = \begin{pmatrix} \frac{bi-a}{1+a} & \frac{1}{1+a} \\ 1 & 0 \end{pmatrix},$$

where parameters a, b, σ and ω are as in Scheme 4. The eigenvalues μ of matrix G satisfy

$(a+1)\mu^2 + (a - bi)\mu - 1 = 0$. The Schur criterion requires for $|\mu| < 1$,

$$d_2 = |(-1)(a - bi) - (a+1)(a+bi)| = a\sqrt{(a+2)^2 + b^2} < d_1,$$

with $d_1 = (a+1)^2 - 1 = a(a+2) > 0$. But obviously we have $d_2 > d_1$ for $\Delta x,\ \Delta t > 0$! Therefore the scheme 4a is unstable (note that the condition $d_2 < d_1$ is also necessary in the Schur criterion).

Scheme 5 (Richtmyer and Morton [8, p.190], No's.10 and 11)

$$(1+\theta)\frac{f_n^{j+2} - f_n^{j+1}}{\Delta t} - \theta\frac{f_n^{j+1} - f_n^j}{\Delta t} = \frac{D(f_n^{j+1})}{\Delta x^2}\delta^2 f_n^{j+2} + C(f_n^{j+1}, \frac{\delta f_n^{j+1}}{2\Delta x}) \tag{18}$$

For the linear model equation (2), we obtain

$$(1 + \theta - \sigma\delta^2) f_n^{j+2} = (2\theta + 1 + \omega\delta) f_n^{j+1} - \theta f_n^j \tag{19}$$

where the parameter θ is a constant, $\sigma = D\Delta t/\Delta x^2$ and $\omega = Dk\Delta t/2\Delta x$.

THEOREM 5 *Scheme 5 for equation (2), i.e. (19), is A-stable if either*

$$\Delta t < \begin{cases} 2(1+2\theta) & \textit{when} \quad -\frac{1}{2} < \theta < 0 \\ 2/(1+2\theta) & \textit{when} \quad \theta \geq 0 \end{cases}$$

or

$$\Delta t < \frac{1}{Dk^2} - \frac{\Delta x^2}{12D} \quad \textit{when} \quad \theta = \frac{1}{2} + \frac{\Delta x^2}{12D\Delta t}.$$

Proof. The amplification matrix for (19) is given by

$$G(\xi, \Delta t) = \begin{pmatrix} \frac{1+2\theta+bi}{1+\theta+a} & -\frac{\theta}{1+\theta+a} \\ 1 & 0 \end{pmatrix},$$

with its eigenvalues μ satisfying the quadratic equation

$$(1 + \theta + a)\mu^2 - (1 + 2\theta + bi)\mu + \theta = 0, \tag{20}$$

where $a = 4\sigma \sin^2 \frac{\xi}{2}$ and $b = 2\omega \sin \xi$. Applying the Schur criterion gives rise to the requirement (see Appendix)

$$\begin{aligned} d_2 &= |\theta(1 + 2\theta + bi)(-1) - (1 + \theta + a)(bi - 1 - 2\theta)| \\ &= \sqrt{(1 + a)^2(1 + 2\theta)^2 + b^2(1 + 2\theta + a)^2} \ < \ d_1 \end{aligned} \tag{21}$$

where $d_1 = (1 + \theta + a)^2 - \theta^2 = (1 + 2\theta + a)(a + 1) > 0$ if $\theta \geq -\frac{1}{2}$. Now the inequality (21) may be written as

$$(\frac{1 + 2\theta}{1 + 2\theta + a})^2 + (\frac{b}{1 + a})^2 < 1 \tag{22}$$

which obviously holds for $k = 0$ and $\xi \neq 0$ *i.e.* $b = 0$ and $a > 0$ (see Richtmyer and Morton [8, p.190]). Consider inequality (22) when $b \neq 0$. It is equivalent to

$$\frac{b^2}{(1 + a)^2} < \frac{a[2(1 + 2\theta) + a]}{(1 + 2\theta + a)^2}$$

i.e.

$$\frac{b^2}{a} < (\frac{1+a}{1+2\theta+a})^2[2(1+2\theta)+a]. \tag{23}$$

Let us first look at the right hand side of (23) in search of its lower bound. Since the following can be verified

$$(\frac{1+a}{1+2\theta+a})^2 \geq \min\{1,\ 1/(1+2\theta)^2\}, \tag{24}$$

therefore the right hand side of (23) is bounded from below by

$$(\frac{1+a}{1+2\theta+a})^2[2(1+2\theta)+a] \geq \begin{cases} a, & & \theta = -\frac{1}{2} \\ 2(1+2\theta)+a & \geq\ 2(1+2\theta), & \theta \in (-\frac{1}{2},0) \\ (2(1+2\theta)+a)/(1+2\theta)^2 & \geq\ 2/(1+2\theta), & \theta \geq 0. \end{cases} \tag{25}$$

Secondly the left hand side of (23) has the upper bound (refer to the proof of Theorem 2)

$$\frac{b^2}{a} = \frac{D^2k^2\Delta t^2 \sin^2\xi}{\Delta x^2}\frac{\Delta x^2}{4D\Delta t\sin^2\frac{\xi}{2}} = \frac{Dk^2\Delta t\sin^2\xi}{4\sin^2\frac{\xi}{2}}$$

$$= Dk^2\Delta t\cos^2\frac{\xi}{2}\ \leq\ Dk^2\Delta t. \tag{26}$$

Combining (25) and (26), we obtain a sufficient condition for inequality (23) to hold :

$$Dk^2\Delta t < \begin{cases} 2(1+2\theta), & \theta \in (-\frac{1}{2},0), \\ 2/(1+2\theta), & \theta \geq 0, \end{cases}$$

i.e.

$$\Delta t < \begin{cases} 2(1+2\theta)/Dk^2, & \theta \in (-\frac{1}{2}, 0), \\ 2/[(1+2\theta)Dk^2], & \theta \geq 0. \end{cases} \tag{27}$$

In particular when $\theta = \frac{1}{2} + \frac{\Delta x^2}{12D\Delta t}$, we have from the second inequality of (27)

$$\Delta t(2 + \frac{\Delta x^2}{6D\Delta t}) < \frac{2}{Dk^2}, \quad i.e. \quad \Delta t < \frac{1}{Dk^2} - \frac{\Delta x^2}{12D}.$$

This completes the proof. □

We comment here that $\theta = \frac{1}{2}$ is the special case as introduced in Scheme 2 while the choice $\theta = \frac{1}{2} + \frac{\Delta x^2}{12D\Delta t}$ increases the order of the truncation error of the scheme. For example, when $k = 0$, Scheme 5 with the latter choice of θ has the accuracy of $O(\Delta t^2) + O(\Delta x^4)$; while the choice $\theta = \frac{1}{2}$ corresponds to $O(\Delta t^2) + O(\Delta x^2)$. See Richtmyer and Morton [8, Ch.8].

3 An explicit three level scheme

This fully explicit scheme due to Du Fort and Frankel [2] is now generalized to solve equation (1) as follows (see Richtmyer and Morton [8, p.190, No.8]).

Scheme 6 (Du Fort and Frankel [2])

$$\frac{f_n^{j+2} - f_n^j}{2\Delta t} = \frac{D(f_n^{j+1})}{\Delta x^2}(f_{n+1}^{j+1} + f_{n-1}^{j+1} - f_n^{j+2} - f_n^j) + C(f_n^{j+1}, \frac{\delta f_n^{j+1}}{2\Delta x}) \tag{28}$$

For the linear model equation (2), we obtain

$$(1+\sigma)f_n^{j+2} = (\sigma\bar{\delta} + \omega\delta)f_n^{j+1} + (1-\delta)f_n^j \tag{29}$$

where $\sigma = 2D\Delta t/\Delta x^2$, $\omega = Dk\Delta t/\Delta x$ and $\bar{\delta} f_n^{j+1} = f_{n+1}^{j+1} + f_{n-1}^{j+1}$.

THEOREM 6 *Scheme 6 for equation (2), i.e. (29), is A-stable if*

$$\Delta t < \frac{\Delta x}{D|k|}.$$

Proof. The eigenvalues μ of the amplification matrix

$$G(\xi, \Delta t) = \begin{pmatrix} \frac{\sigma_1 + bi}{1+\sigma} & \frac{1-\sigma}{1+\sigma} \\ 1 & 0 \end{pmatrix}$$

for (29) satisfy the quadratic equation

$$(1+\sigma)\mu^2 - (\sigma_1 + bi)\mu + (\sigma - 1) = 0, \tag{30}$$

where $\sigma_1 = 2\sigma\cos\xi$ and $b = 2\omega\sin\xi$. We use the Schur criterion, requiring

$$d_2 = |(\sigma-1)(-\sigma_1 - bi) - (\sigma+1)(-\sigma_1 + bi)| = 4\sigma\sqrt{\cos^2\xi + \omega^2\sin^2\xi} < d_1 = 4\sigma.$$

Provided that $\sigma \neq 0$ (*i.e.* $\xi \neq 0$), this adds up to requiring $|\omega| < 1$. Hence $|Dk\Delta t/\Delta x| < 1$ *i.e.* $\Delta t < \Delta x/(D|k|)$ offers a sufficient condition. □

Although the stepsize restriction here is the same as that for Schemes 1 and 4, the accuracy of the scheme requires that Δt be much smaller than Δx (refer to §5).

4 The modified Varah scheme

All the above discussed schemes, evaluating the lower order terms in the space derivatives at the intermediate level $j+1$, may be classified as 'leap-frog' schemes. The following scheme due to Varah [12] uses 'equal weighting' for all terms in (1) (compare with Scheme 5)

$$(\frac{1}{2}+\theta_1)\frac{f_n^{j+2}-f_n^{j+1}}{\Delta t}+(\frac{1}{2}-\theta_1)\frac{f_n^{j+1}-f_n^j}{\Delta t}=\frac{D(f_n^{j+1})}{\Delta x^2}\delta^2\bar{f}_n^{j+1}+C(\bar{f}_n^{j+1},\frac{\bar{f}_n^{j+1}}{2\Delta x}) \tag{31}$$

where $-1 \leq \theta_1 \leq 1$ and $\bar{f}_n^{j+1} = \theta_1 f_n^{j+2} + (1-\theta_1)f_n^{j+1}$. To see the relationship of (31) with previous schemes, say Scheme 5, let us denote $\theta = \theta_1 - \frac{1}{2}$. Then formula (31) then may be written in an equivalent form

$$(1+\theta)\frac{f_n^{j+2}-f_n^{j+1}}{\Delta t}-\theta\frac{f_n^{j+1}-f_n^j}{\Delta t}=\frac{D(f_n^{j+1})}{\Delta x^2}\delta^2\hat{f}_n^{j+1}+C(\hat{f}_n^{j+1},\frac{\delta\hat{f}_n^{j+1}}{2\Delta x}) \tag{32}$$

where $\hat{f}_n^{j+1} = (\frac{1}{2}+\theta)f_n^{j+2} + (\frac{1}{2}-\theta)f_n^{j+1}$ with $-\frac{3}{2} \leq \theta \leq \frac{1}{2}$. Now the above scheme differs from Scheme 5 only in approximating the right hand side of equation (1).

However in general equation (32) is nonlinear in f_n^{j+2}. Therefore the advantage of a three level scheme is not present. One partially linearized version of (32) is given in Varah [12] but we still have the problem of having to solve a nonlinear system in some cases. Below we propose to linearize (32) based on an idea from Richtmyer and Morton [8, Ch.8].

From Taylor's Theorem, we have the expansion

$$C(u,v) = C(u,v_0) + C_v(u,v_0)(v-v_0) + O((v-v_0)^2) \tag{33}$$

Therefore taking $u = \bar{f}_n^{j+1}$ and $v_0 = \frac{\delta f_n^{j+1}}{2\Delta x}$, we can replace (32) by the following

Scheme 7 (Linearization of Varah [12])

$$\begin{aligned}(1+\theta)\frac{f_n^{j+2}-f_n^{j+1}}{\Delta t} - \theta\frac{f_n^{j+1}-f_n^j}{\Delta t} &= \frac{D(f_n^{j+1})}{\Delta x^2}\delta^2\hat{f}_n^{j+1} + C(\bar{f}_n^{j+1}, \frac{\delta f_n^{j+1}}{2\Delta x}) \\ &+ (\frac{1}{2}+\theta)C_v(\bar{f}_n^{j+1}, \frac{\delta f_n^{j+1}}{2\Delta x})(\frac{\delta f_n^{j+2}}{2\Delta x} - \frac{\delta f_n^{j+1}}{2\Delta x}), \end{aligned} \tag{34}$$

where $\bar{f}_n^{j+1} = (\frac{3}{2}+\theta)f_n^{j+1} - (\frac{1}{2}+\theta)f_n^j$. For example, when $C(f, \frac{\partial f}{\partial x}) = \bar{C}(f)(\frac{\partial f}{\partial x})^2$ *i.e.* $C(u,v) = \bar{C}(u)v^2$, equation (34) of Scheme 7 is simplified to

$$\begin{aligned}&(1+\theta)\frac{f_n^{j+2}-f_n^{j+1}}{\Delta t} - \theta\frac{f_n^{j+1}-f_n^j}{\Delta t} \\ &= \frac{D(f_n^{j+1})}{\Delta x^2}\delta^2\hat{f}_n^{j+1} + \bar{C}(\bar{f}_n^{j+1})\frac{\delta f_n^{j+1}}{2\Delta x}[(1+2\theta)\frac{\delta f_n^{j+2}}{2\Delta x} - 2\theta\frac{\delta f_n^{j+1}}{2\Delta x}].\end{aligned} \tag{35}$$

For the linear model equation (2), we obtain from (34)

$$[(1+\theta) - (\frac{1}{2}+\theta)(\sigma\delta^2 + \omega\delta)]f_n^{j+2} = [(1+2\theta) + (\frac{1}{2}-\theta)(\sigma\delta^2+\omega\delta)]f_n^{j+1} - \theta f_n^j \quad (36)$$

with $\sigma = D\Delta t/\Delta x^2$ and $\omega = Dk\Delta t/2\Delta x$.

THEOREM 7 *Scheme 7 for equation (2), i.e. (36), is A-stable if* $0 \le \theta \le \frac{1}{2}$.

Proof. Along similar lines of proving Theorems 1–6, refer to Varah [12]. □

Remark 1. When $\theta = \frac{1}{2}$, Scheme 7 takes the form

$$\begin{aligned} \frac{3}{2}\frac{f_n^{j+2}-f_n^{j+1}}{\Delta t} - \frac{1}{2}\frac{f_n^{j+1}-f_n^j}{\Delta t} &= \frac{D(f_n^{j+1})}{\Delta x^2}\delta^2 f_n^{j+2} + C(\bar{f}_n^{j+1}, \frac{\delta f_n^{j+1}}{2\Delta x}) \\ &+ C_v(\bar{f}_n^{j+1}, \frac{\delta f_n^{j+1}}{2\Delta x})(\frac{\delta f_n^{j+2}}{2\Delta x} - \frac{\delta f_n^{j+1}}{2\Delta x}), \end{aligned} \quad (37)$$

where $\bar{f}_n^{j+1} = 2f_n^{j+1} - f_n^j$. Equation (37) is almost identical to Scheme 2 of (7) but the difference is again in approximating lower order terms in the spatial derivatives of (1).

Remark 2. In our Scheme 7, the introduction of quantity $\bar{f}_n^{j+1}$ is due to Varah [12] but his linearization does not extend to terms involving $\frac{\partial f}{\partial x}$.

Remark 3. It should be noted that all schemes presented are A-stable for the following model diffusion equation

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2}.$$

Refer to Mitchell and Griffiths [7], Richtmyer and Morton [8] and Smith [9]. Therefore we shall not test this simple model equation.

Remark 4. One interesting, and also important, point is that the stability analysis for Schemes 1, 3, 4, 6 and 7 uses the assumption that $\xi = \beta \Delta x > 0$. Therefore the possibility that one of the eigenvalues satisfies $|\mu| = 1$ exists for these schemes. This may lead to oscillatory solutions. See Varah [12] for one example. However Scheme 5 with a general θ (including Scheme 2) does not possess such a problem. That is, $|\mu| < 1$ strictly when the stability condition is met.

5 Local error analysis

The local accuracies of these seven schemes are given by the following theorem.

THEOREM 8 *For our linear model equation (2), i.e.,*

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2} + Dk \frac{\partial f}{\partial x}$$

with exact solution F, we define the local truncation error of a scheme such as (3) by

$$T(F)_n^{j+1} = \frac{1}{\Delta t} \sum_{\ell=0}^{2} w_\ell F_n^{j+\ell} - \frac{D}{\Delta x^2} \sum_{\ell=0}^{2} \sum_{m=-1}^{1} \bar{w}_\ell^{(m)} F_{n+m}^{j+\ell} - C\left(\sum_{\ell=0}^{2} \tilde{w}_\ell F_n^{j+\ell}, \frac{1}{\Delta x} \sum_{\ell=0}^{2} \hat{w}_\ell F_n^{j+\ell} \right). \tag{38}$$

Then for the schemes presented so far, we have for

$$
\begin{array}{llllll}
\underline{\textit{Scheme 1}} & T(F)_n^{j+1} = & R_1^{(1)}\Delta t & + R_1^{(2)}\Delta t^2 & + R_1^{(3)}\Delta x^2 & + \cdots \\
\underline{\textit{Scheme 2}} & T(F)_n^{j+1} = & R_2^{(1)}\Delta t & + R_2^{(2)}\Delta t^2 & + R_2^{(3)}\Delta x^2 & + \cdots \\
\underline{\textit{Scheme 3}} & T(F)_n^{j+1} = & & R_3^{(2)}\Delta t^2 & + R_3^{(3)}\Delta x^2 & + \cdots \\
\underline{\textit{Scheme 4}} & T(F)_n^{j+1} = & & R_4^{(2)}\Delta t^2 & + R_4^{(3)}\Delta x^2 & + \cdots \\
\underline{\textit{Scheme 5}} & T(F)_n^{j+1} = & R_5^{(1)}\Delta t & + R_5^{(2)}\Delta t^2 & + R_5^{(3)}\Delta x^2 & + \cdots \\
\underline{\textit{Scheme 6}} & T(F)_n^{j+1} = & R_6^{(1)}(\frac{\Delta t}{\Delta x})^2 & + R_6^{(2)}\Delta t^2 & + R_6^{(3)}\Delta x^2 & + \cdots \\
\underline{\textit{Scheme 7}} & T(F)_n^{j+1} = & & R_7^{(2)}\Delta t^2 & + R_7^{(3)}\Delta x^2 & + \cdots
\end{array}
$$

where

$$
\left\{
\begin{array}{lll}
R_1^{(1)} & = & -D(\frac{\partial^3 F}{\partial x^2 \partial t})_n^{j+1} \\
R_1^{(2)} & = & \frac{1}{6}(\frac{\partial^3 F}{\partial t^3})_n^{j+1} - \frac{D}{4}(\frac{\partial^4 F}{\partial x^2 \partial t^2})_n^{j+1} \\
R_1^{(3)} & = & -\frac{Dk}{6}(\frac{\partial^3 F}{\partial x^3})_n^{j+1} - \frac{D}{12}(\frac{\partial^4 F}{\partial x^4})_n^{j+1}
\end{array}
\right.
$$

$$
\left\{
\begin{array}{lll}
R_2^{(1)} & = & Dk(\frac{\partial^2 F}{\partial x \partial t})_n^{j+1} \\
R_2^{(2)} & = & R_1^{(2)} \\
R_2^{(3)} & = & R_1^{(3)}
\end{array}
\right.
$$

$$
\left\{
\begin{array}{lll}
R_3^{(2)} & = & \frac{1}{6}(\frac{\partial^3 F}{\partial t^3})_n^{j+1} - \frac{D}{6}(\frac{\partial^4 F}{\partial x^2 \partial t^2})_n^{j+1} \\
R_3^{(3)} & = & -\frac{Dk}{6}(\frac{\partial^3 F}{\partial x^3})_n^{j+1} - \frac{D}{18}(\frac{\partial^4 F}{\partial x^4})_n^{j+1}
\end{array}
\right.
$$

$$\begin{cases} R_4^{(2)} &= R_1^{(2)} \\ R_4^{(3)} &= R_1^{(3)} \end{cases}$$

$$\begin{cases} R_5^{(1)} &= D^2 \frac{\partial^2}{\partial x^2}[(\theta - \frac{1}{2})\frac{\partial^2 F}{\partial x^2} + 2\theta k \frac{\partial F}{\partial x} + k^2 F]_n^{j+1} \\ R_5^{(2)} &= R_1^{(2)} \\ R_5^{(3)} &= R_1^{(3)} \end{cases}$$

$$\begin{cases} R_6^{(1)} &= D(\frac{\partial^2 F}{\partial t^2})_n^{j+1} \\ R_6^{(2)} &= \frac{1}{6}(\frac{\partial^3 F}{\partial t^3})_n^{j+1} \\ R_6^{(3)} &= R_1^{(3)} \end{cases}$$

$$\begin{cases} R_7^{(2)} &= R_1^{(2)} + \frac{D}{4}(\frac{1}{2} - \theta)(\frac{\partial^4 F}{\partial x^4})_n^{j+1} - \frac{Dk}{2}(\frac{1}{2} + \theta)(\frac{\partial^3 F}{\partial x \partial x^2})_n^{j+1} \\ R_7^{(3)} &= R_1^{(3)} \end{cases}$$

with $F_n^{j+1} = F(n\Delta x, (j+1)\Delta t)$. Obviously Scheme 5 (including Scheme 2 as a special case of $\theta = \frac{1}{2}$) has a second order accuracy *i.e.* $R_5^{(1)} = 0$ if the exact solution F satisfies the equation

$$(\theta - \frac{1}{2})\frac{\partial^2 F}{\partial x^2} + 2\theta k \frac{\partial F}{\partial x} + k^2 F = 0. \tag{39}$$

Proof. Using Taylor's Theorem, we can obtain the following :

1) $\frac{F_n^{j+2} - F_n^j}{2\Delta t} = (\frac{\partial F}{\partial t})_n^{j+1} + \frac{\Delta t^2}{6}(\frac{\partial^3 F}{\partial t^3})_n^{j+1} + \cdots$

2) $(1+\theta)\frac{F_n^{j+2} - F_n^{j+1}}{\Delta t} - \theta \frac{F_n^{j+1} - F_n^j}{\Delta t}$

$= (\frac{\partial F}{\partial t})_n^{j+1} + (\frac{1}{2} + \theta)\Delta t(\frac{\partial^2 F}{\partial t^2})_n^{j+1} + \frac{\Delta t^2}{6}(\frac{\partial^3 F}{\partial t^3})_n^{j+1} + \cdots$

3) $\frac{\delta F_n^{j+2}}{2\Delta x} = (\frac{\partial F}{\partial x})_n^{j+1} + \Delta t(\frac{\partial^2 F}{\partial x \partial t})_n^{j+1} + \frac{\Delta t^2}{2}(\frac{\partial^3 F}{\partial x \partial t^2})_n^{j+1} + \frac{\Delta x^2}{6}(\frac{\partial^3 F}{\partial x^3})_n^{j+1} + \cdots$

4) $\frac{\delta F_n^{j+1}}{2\Delta x} = (\frac{\partial F}{\partial x})_n^{j+1} + \frac{\Delta x^2}{6}(\frac{\partial^3 F}{\partial x^3})_n^{j+1} + \cdots$

5) $\frac{\delta^2 F_n^{j+2}}{\Delta x^2} = (\frac{\partial^2 F}{\partial x^2})_n^{j+1} + \Delta t(\frac{\partial^3 F}{\partial x^2 \partial t})_n^{j+1} + \frac{\Delta t^2}{4}(\frac{\partial^4 F}{\partial x^2 \partial t^2})_n^{j+1} + \frac{\Delta x^2}{12}(\frac{\partial^4 F}{\partial x^4})_n^{j+1} + \cdots$

6) $\frac{\delta^2 F_n^{j+1}}{\Delta x^2} = (\frac{\partial^2 F}{\partial x^2})_n^{j+1} + \frac{\Delta x^2}{12}(\frac{\partial^4 F}{\partial x^4})_n^{j+1} + \cdots$

7) $\frac{\delta^2 F_n^{j}}{\Delta x^2} = (\frac{\partial^2 F}{\partial x^2})_n^{j+1} - \Delta t(\frac{\partial^3 F}{\partial x^2 \partial t})_n^{j+1} + \frac{\Delta t^2}{4}(\frac{\partial^4 F}{\partial x^2 \partial t^2})_n^{j+1} + \frac{\Delta x^2}{12}(\frac{\partial^4 F}{\partial x^4})_n^{j+1} + \cdots$

8) $\frac{F_{n+1}^{j+1} + F_{n-1}^{j+1} - F_n^{j+2} - F_n^{j}}{\Delta x^2} = (\frac{\partial^2 F}{\partial x^2})_n^{j+1} - (\frac{\Delta t}{\Delta x})^2(\frac{\partial^2 F}{\partial t^2})_n^{j+1} + \frac{\Delta x^2}{12}(\frac{\partial^4 F}{\partial x^4})_n^{j+1} + \cdots$

On substituting these quantities into schemes 1-7, we complete the proof. □

6 Test examples and experiments

We shall experiment on four test equations of the form (1) as well as on the linear model (2). Our prime purpose is to examine the practical stability of the seven schemes presented and the adequacy or otherwise of the linear stability theory.

6.1 Model 1 — Linear model equation

We here specify equation (2) further by taking $D = 1$ and $k = 1$, so that

$$\frac{\partial f}{\partial t} = \frac{\partial^2 f}{\partial x^2} + \frac{\partial f}{\partial x} \tag{40}$$

for $0 \leq x \leq 1$. We use the following initial condition and boundary conditions

$$\begin{cases} f(x,0) &= \exp[-200(x-\frac{1}{4})^2], \\ \partial f/\partial x &= 0, \qquad (x = 0, 1). \end{cases} \tag{41}$$

As is well known, the solution is a travelling and diffusing wave with reflections from boundaries.

6.2 Model 2 — Nonlinear model equation (1)

Here we take $D = 1$ and $C = (\frac{\partial f}{\partial x})^2$ in equation (1), giving a nonlinear model equation

$$\frac{\partial f}{\partial t} = \frac{\partial^2 f}{\partial x^2} + (\frac{\partial f}{\partial x})^2 \tag{42}$$

for which the solution away from boundaries exhibits a smoothed corner singularity with the conditions of (41).

6.3 Model 3 — Nonlinear model equation (2)

We now vary the diffusion coefficient D in (1) by taking $D = 1 + f$ and $C = \frac{\partial f}{\partial x}$, giving another nonlinear model equation

$$\frac{\partial f}{\partial t} = (1 + f)\frac{\partial^2 f}{\partial x^2} + \frac{\partial f}{\partial x} \tag{43}$$

We again use the conditions of (41). The solution away from boundaries is a travelling wave with nonlinear diffusion.

6.4 Model 4 — Nonlinear Burgers' equation (3)

We take one example of the Burgers' equation (with γ =0.01)

$$\frac{\partial f}{\partial t} = \gamma \frac{\partial^2 f}{\partial x^2} - f \frac{\partial f}{\partial x} \tag{44}$$

which corresponds to taking $D = \frac{1}{100}$ and $C = -f\frac{\partial f}{\partial x}$ in equation (1). The exact solution of (44) is given by (see Whitham [13])

$$f(x,t) = 1 - \frac{9r_1 + 5r_2}{10(r_1 + r_2 + r_3)}, \tag{45}$$

where

$$\begin{aligned} r_1 &= \exp\{-[(x - \tfrac{1}{2})/20\gamma] - 99t/400\gamma\} \\ r_2 &= \exp\{-[(x - \tfrac{1}{2})/4\gamma] - 3t/16\gamma\} \\ r_3 &= \exp\{-[(x - \tfrac{3}{8})/2\gamma] \end{aligned}$$

The example has been used in Varah [12].

6.5 Model 5 — Nonlinear model equation (4)

We now vary coefficients D and C in (1) by taking $D = 1 + f$ and $C = (\frac{\partial f}{\partial x})^2$, giving the fully nonlinear model equation

$$\frac{\partial f}{\partial t} = (1+f)\frac{\partial^2 f}{\partial x^2} + (\frac{\partial f}{\partial x})^2 \qquad \left(= \frac{\partial}{\partial x}\{(1+f)\frac{\partial f}{\partial x}\}\right) \tag{46}$$

the solution of which has a smoothed corner discontinuity and, with the conditions of (41), exhibits behaviour similar to that found in semiconductor process modelling profiles. Refer to Smyth and Hill [10].

Following §2–5, we now tabulate in Table i the theoretical stability restrictions upon Δt, given Δx. In our numerical calculations we choose two particular stepsizes $\Delta x_1 = 10^{-2}$ and $\Delta x_2 = 2\times 10^{-3}$. Numerical stability conditions observed from testing on our examples are listed in Table ii. For Scheme 5, we take $\theta = \frac{1}{2} + \frac{\Delta x^2}{12D\Delta t}$ and for Scheme 7 $\theta = \frac{1}{2}$. Our experiments are carried out on a SUN 3/60 computer.

In Table ii the entry of ∞ means that no restriction on time stepsize Δt is observed for that particular case. We can see that results of Table ii are well predicted by Table i. In particular, Schemes 2 and 5 as well as Scheme 7 do not have any time stepsize restriction for the fully nonlinear example 5. However Scheme 7 has a second order accuracy in both time and space while Schemes 2 and 5 have a second order accuracy in space but a first order accuracy in time in general. The latter can only have a second order accuracy in time when the exact solution satisfies equation (39).

7 Conclusions

Here we have proposed seven time discretization schemes of three-level type and analyzed their linear stability as well as local error estimates. We have shown that Schemes 2, 5 and 7 are better than other 'leap-frog' schemes (including Scheme 4 used in [11]) in terms of stability. In particular Scheme 7 is unconditionally stable whilst the restriction on Schemes 2 and 5 is not severe. Comparison of Scheme 7 with Schemes 2 and 5 shows that one of the eigenvalues of amplification matrix of the former may have modulus one while the latter schemes do not have such a problem.

Numerical results have shown that Schemes 2 and 5 behave closely to Scheme 7 in terms of stability and accuracy, particularly for the fully nonlinear example 5. High order schemes based on the 'leap-frog' idea (such as Scheme 4) do not have good stability conditions. The implicit treatment of the first order spatial derivative term is evidently important for improving stability. The more implicitly we treat these terms, the more stable our schemes will be. Generally speaking, Schemes 1, 2, 5 and 7 are comparable although Scheme 7 is the most robust and reliable.

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Appendix — The Schur criterion

This criterion was investigated in great detail by Miller [6].

Suppose that a quadratic equation is expressed as

$$c_2\mu^2 + c_1\mu + c_0 = 0 \tag{47}$$

where c_j's are in general complex numbers. Then the roots of (47) satisfy $|\mu| < 1$ if and only if

$$\left.\begin{aligned} &\textbf{1)}\quad d_1 = |c_2|^2 - |c_0|^2 > 0, \\ &\textbf{2)}\quad d_2 = |c_2^* c_1 - c_0 c_1^*| < d_1, \end{aligned}\right\} \tag{48}$$

where '*' represents the conjugate of a complex number. Now since $|c_2^* c_1 - c_0 c_1^*| = |c_0^* c_1 - c_2 c_1^*|$, then conditions of (48) can be replaced by

$$\left.\begin{aligned} &\textbf{a)}\quad d_1 = |c_2|^2 - |c_0|^2 > 0, \\ &\textbf{b)}\quad d_2 = |c_0^* c_1 - c_2 c_1^*| < d_1. \end{aligned}\right\} \tag{49}$$

In Lambert [5, p.78], (48) is referred to as the Schur-Wilf criterion when the coefficients c_j's in (47) are real; whilst in Henrici [4, p.494], (49) is called the Schur-Cohn criterion.

Figure 1: Time step advance in a three-level scheme

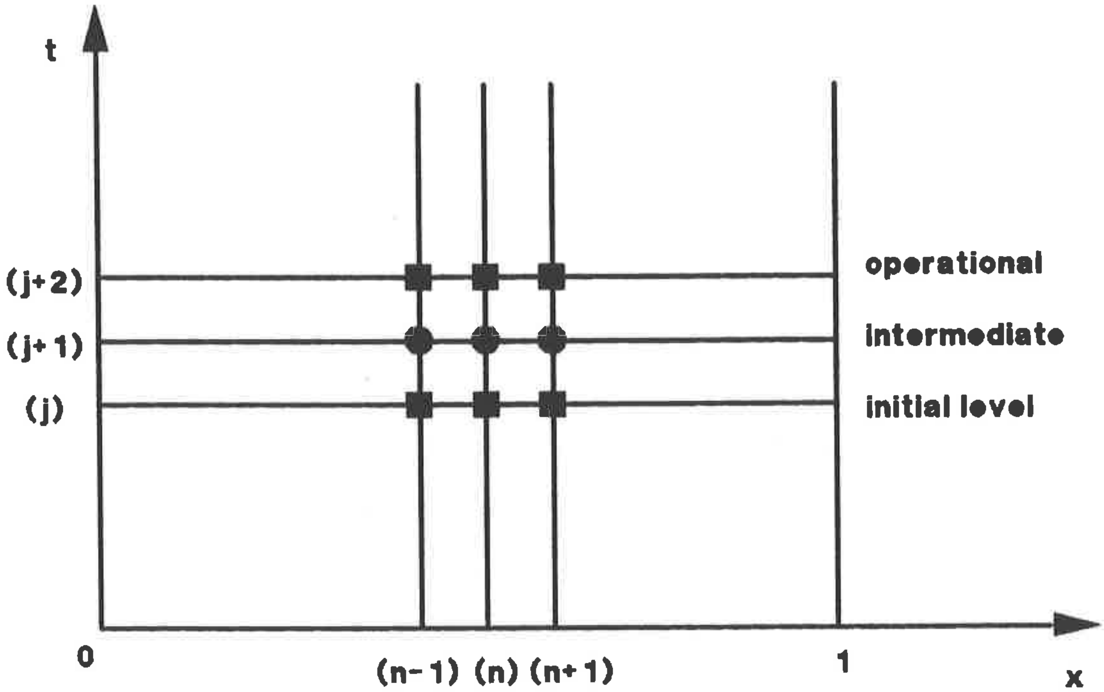

Table i: Theoretical restriction on Δt from the linear stability analysis

Model Problem	Numerical Scheme	Theoretical Restriction ($\Delta t <$)
1 (D=k=1)	1	Δx
	2	1
	3	$\frac{\sqrt{3}}{2}\Delta x$
	4	Δx
	5	$1 - \frac{\Delta x^2}{12}$
	6	Δx
	7	∞
2 (D=1) (k=$\frac{\partial f}{\partial x}$)	1	$\Delta x/\lvert k\rvert$
	2	$1/k^2$
	3	$\frac{\sqrt{3}}{2}\Delta x/\lvert k\rvert$
	4	$\Delta x/\lvert k\rvert$
	5	$1/k^2 - \frac{\Delta x^2}{12}$
	6	$\Delta x/\lvert k\rvert$
	7	∞
3 (D=1+f) (k=1/D)	1	Δx
	2	D
	3	$\frac{\sqrt{3}}{2}\Delta x$
	4	Δx
	5	$D - \frac{\Delta x^2}{12D}$
	6	Δx
	7	∞
4 (D=0.01) (k=−100f)	1	$\Delta x/\lvert f\rvert$
	2	$0.01/f^2$
	3	$\frac{\sqrt{3}}{2}\Delta x/\lvert f\rvert$
	4	$\Delta x/\lvert f\rvert$
	5	$0.01/f^2 - 100\frac{\Delta x^2}{12}$
	6	$\Delta x/\lvert f\rvert$
	7	∞
5 (D=1+f) (k=$\frac{\partial f}{\partial x}/D$)	1	$\Delta x/\lvert\frac{\partial f}{\partial x}\rvert$
	2	$D/(\frac{\partial f}{\partial x})^2$
	3	$\frac{\sqrt{3}}{2}\Delta x/\lvert\frac{\partial f}{\partial x}\rvert$
	4	$\Delta x/\lvert\frac{\partial f}{\partial x}\rvert$
	5	$D/(\frac{\partial f}{\partial x})^2 - \frac{\Delta x^2}{12D}$
	6	$\Delta x/\lvert\frac{\partial f}{\partial x}\rvert$
	7	∞

Table ii: Observed restriction on time step Δt from numerical experiments

Model Problem (Number)	Numerical Scheme (Number)	Theoretical Restriction ($\Delta t <$) (Δx_1 =1.E-2)	(Δx_2 =2.E-3
1 (D=k=1)	1	∞	4.E-3
	2	∞	∞
	3	5.E-3	1.E-3
	4	1.E-3	1.E-3
	5	∞	∞
	6	3.E-4	1.E-5
	7	∞	∞
2 (D=1) (k=$\frac{\partial f}{\partial x}$)	1	1.E-2	5.E-3
	2	1.E-2	5.E-3
	3	1.E-4	1.E-4
	4	1.E-4	1.E-4
	5	5.E-2	1.E-2
	6	1.E-4	1.E-5
	7	∞	∞
3 (D=1+f) (k=1/D)	1	∞	∞
	2	∞	∞
	3	5.E-4	1.E-4
	4	5.E-4	1.E-4
	5	∞	∞
	6	1.E-2	1.E-2
	7	∞	∞
4 (D=0.01) (k=−100f)	1	1.E-2	1.E-2
	2	1.E-2	1.E-2
	3	1.E-2	1.E-2
	4	1.E-2	1.E-2
	5	2.E-2	1.E-2
	6	1.E-2	1.E-4
	7	∞	∞
5 (D=1+f) (k=$\frac{\partial f}{\partial x}/D$)	1	1.E-2	1.E-3
	2	∞	∞
	3	1.E-4	1.E-4
	4	1.E-4	1.E-4
	5	∞	∞
	6	1.E-4	1.E-5
	7	∞	∞