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NOTE

On the Conditional Consistency of an Explicit Numerical Scheme

1. INTRODUCTION

In this paper we analyse an explicit scheme for the solution of partial differential equations, recently presented in this Journal by Richardson, Ferrel, and Long [4]; these authors presented the algorithm as an unconditionally stable explicit scheme for solving non-linear fluid dynamics problems.

The present study, with application to the one-dimensional diffusion equation, shows that the scheme is indeed unconditionally stable, but only conditionally consistent.

As a simple example of this problem, it is enough to remember the unconditionally stable DuFort–Frankel discretization [1] of the one-dimensional linear diffusion equation (parabolic), which can become consistent with a hyperbolic equation if, when Δt and Δx approach zero, the ratio $\Delta t/\Delta x$ tends to a greater-than-zero constant value.

Besides, for the scheme here analysed, since the modulus of the amplification factor is almost constant for Δt larger than a certain value, the convergence properties of the scheme do not improve for large values of Δt.

Finally, if one tries to perform the integration with very high time step values, perturbations can be introduced in the transient phase because of the difference equation inconsistency; this is shown by the numerical examples.

2. THE RICHARDSON–FERREL–LONG SCHEME

In the following section we recall the scheme developed by Richardson *et al.* [2–4], which is an explicit finite difference scheme, second-order accurate in space (central discretization); it has, in the actual formulation, a first-order time accuracy.

Let us consider the one-dimensional linear diffusion equation (ν is a positive constant)

$$\frac{\partial u}{\partial t}(x, t) = \nu \frac{\partial^2 u}{\partial x^2}(x, t). \tag{1}$$

By using a second-order spatial discretization we get its space discretized form ($x_i = i\Delta x$ and Δx is the grid size)

$$\frac{du}{dt} = \frac{\nu}{\Delta x^2}(u_{i-1} - 2u_i + u_{i+1})$$

or, in vector form

$$\frac{du}{dt} = \frac{\nu}{\Delta x^2}(Lu)$$

with L a tridiagonal matrix operator whose ith row is

$$\dots\ 1\ -2\ 1\ \dots.$$

Equation (1) is formally solved by

$$u(t + \Delta t) = \exp(\alpha L)u(t)$$

with $\alpha = \nu\Delta t/\Delta x^2$.

The approximation technique for the exponential function determines the time integration method; for example, by using the series definition of $\exp(\alpha L)$ and stopping the expansion at the first order, we reach the classical Euler explicit scheme, or by using the rational Padé's approximation [5] for the exp function, we get the well-known Crank–Nicholson (trapezoidal rule) scheme and so on.

The method under discussion has its basis on the decomposition of the L matrix into a sum of two block diagonal matrices where each block can be easily exponentiated (that is, calling A the generic block, the exact expression of $\exp(A)$ can easily be written). So, we can write

$$L = L_e + L_o,$$

where

$$L_e = \begin{bmatrix} -1 & 1 & 0 & 0 & \cdots \\ 1 & -1 & 0 & 0 & \cdots \\ 0 & 0 & -1 & 1 & \cdots \\ 0 & 0 & 1 & -1 & \cdots \\ \vdots & & & & \end{bmatrix};$$

$$L_0 = \begin{bmatrix} -1 & 0 & 0 & 0 & \cdots \\ 0 & -1 & 1 & 0 & \cdots \\ 0 & 1 & -1 & 0 & \cdots \\ 0 & 0 & 0 & -1 & \cdots \\ \vdots & & & & \end{bmatrix}.$$

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Let us remember that if Y and Z are two non-commutative matrices, the product $\exp(Y)\exp(Z)$ is not exactly equal to $\exp(Y+Z)$ [6], but we can write

$$\exp(\alpha L) = \exp[(\alpha L_e) + (\alpha L_o)] = \exp(\alpha L_e)\exp(\alpha L_o) + O(\alpha^2)$$

so that a first-order time step operator follows

$$T = \exp(\alpha L_e)\exp(\alpha L_o)$$

and the updating of the u vector is carried out by the relation

$$u^{(n+1)} = Tu^{(n)}.$$

The next problem is to express the exponential of the following (2×2) block

$$A = \alpha \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$

which is repeated, identically, in the L_e and L_o matrices.

From the series definition for the matrix exponential function

$$\exp(A) = I + \sum_{n=1}^{\infty} \frac{A^n}{n!},$$

observing that

$$A^n = \frac{(-2\alpha)^n}{2} A,$$

we get

$$\exp(A) = I - \sum_{n=1}^{\infty} \frac{(-2\alpha)^n}{2n!} A.$$

By using again the exponential function series definition for each element of the matrix $\exp(A)$, we find

$$\exp(A) = \frac{1}{2}\begin{bmatrix} 1+e^{-2\alpha} & 1-e^{-2\alpha} \\ 1-e^{-2\alpha} & 1+e^{-2\alpha} \end{bmatrix} = \begin{bmatrix} e_1 & e_2 \\ e_2 & e_1 \end{bmatrix},$$

where $2e_1 = 1 + e^{-2\alpha}$ and $2e_2 = 1 - e^{-2\alpha}$.

By applying the $\exp(\alpha L_o)$ semi-operator to $u^{(n)}$, we obtain

$$[\exp(\alpha L_o)u^{(n)}]_i = e_2 D_i u_{i-1} + e_1 u_i + e_2 P_i u_{i+1} = \hat{u}_i, \qquad (2)$$

where D_i and P_i are two operators defined as

$$D_i = \frac{1-(-1)^i}{2}; \quad P_i = \frac{1+(-1)^i}{2}.$$

Then, by applying the semi-operator $\exp(\alpha L_e)$ to $\hat{u}$ we get

$$[\exp(\alpha L_e)\hat{u}]_i = e_2 P_i \hat{u}_{i-1} + e_1 \hat{u}_i + e_2 D_i \hat{u}_{i+1} = u_i^{(n+1)}. \qquad (3)$$

By means of the two previous half steps, it is possible to carry out a single time step.

3. CONDITIONAL CONSISTENCY

The first main requirement of a practically usable scheme is consistency (the difference operator approaches the differential operator when the mesh size tends to zero).

For the validity of the factorization of the $\exp(\alpha L)$ function (Section 2) α must obviously be small $\nu\Delta t < \Delta x^2$. We show *in this section that consistency requires an even more restrictive* condition on Δt (in the following we shall assume that $\nu = 1$). *To verify this property, the modified equation method* [1] is used.

The discrete updating equation is

$$u_i^{(n+1)} = e_2^2 P_i u_{i-2}^{(n)} + e_1 e_2 u_{i-1}^{(n)} + e_1^2 u_i^{(n)} + e_1 e_2 u_{i+1}^{(n)} + e_2^2 D_i u_{i+2}^{(n)},$$

obtained by the substitution of (2) in (3); by writing the Taylor series expansion in time and space around the $u_i^{(n)}$ value, we get

$$\begin{aligned} u + u_t\Delta t + u_{tt}\frac{\Delta t^2}{2!} + \cdots &= e_2^2 P_i \left[u - u_x 2\Delta x + u_{xx}\frac{(2\Delta x)^2}{2!} - u_{xxx}\frac{(2\Delta x)^3}{3!} + \cdots \right] \\ &+ e_1 e_2 \left[u - u_x\Delta x + u_{xx}\frac{\Delta x^2}{2!} - u_{xxx}\frac{\Delta x^3}{3!} + \cdots \right] \\ &+ e_1^2 u \\ &+ e_1 e_2 \left[u + u_x\Delta x + u_{xx}\frac{\Delta x^2}{2!} + u_{xxx}\frac{\Delta x^3}{3!} + \cdots \right] \\ &+ e_2^2 D_i \left[u + u_x 2\Delta x + u_{xx}\frac{(2\Delta x)^2}{2!} + u_{xxx}\frac{(2\Delta x)^3}{3!} + \cdots \right], \end{aligned} \qquad (4)$$

where, for simplicity, subscript i and superscript n in u and in the derivatives were dropped.

The functions e_1^2, e_2^2, and $e_1 e_2$ were expanded by the usual Taylor expression:

$$\begin{aligned} e_2^2 &= \alpha^2 - 2\alpha^3 + O(\alpha^4) \\ e_1^2 &= 1 - 2\alpha + 3\alpha^2 - \frac{20}{6}\alpha^3 + O(\alpha^4) \\ e_1 e_2 &= \alpha - 2\alpha^2 + \frac{16}{6}\alpha^3 + O(\alpha^4). \end{aligned} \qquad (5)$$

By the substitution of (5) in (4), we obtain, after some algebra, the expression for the modified equation,

$$u_t - \nu u_{xx} = (4\alpha^3 \mp 2\alpha^2) u_x \frac{\Delta x}{\Delta t} - \frac{4}{3}\alpha^3 u_{xx}\frac{\Delta x^2}{\Delta t} + \left(\mp\frac{8}{6}\alpha^2 \pm \frac{8}{3}\alpha^3\right) u_{xxx}\frac{\Delta x^3}{\Delta t} + \cdots, \tag{6}$$

where the first or the second sign is to be assumed respectively for even or odd i.

The right-hand side term in (6) represents the truncation error (let us note that the highest time derivative term $u_{tt}\,\Delta t/2$ is missing in it); consistency of the finite difference equation with (1) can be asserted if this tends to zero for Δx and Δt both vanishing, which does not happen for an arbitrary vanishing process. In fact, by analysing the coefficients of (6) it is not difficult to realize that they vanish (for Δx and $\Delta t \to 0$) only if

$$\lim_{\substack{\Delta t\to 0\\ \Delta x\to 0}} \frac{\Delta t}{\Delta x^3} = 0. \tag{7}$$

In other words, in order to let the truncation error reduce to zero when Δx and Δt tend to zero, it is necessary that Δt converges much faster than Δx; in these cases we have conditional consistency.

To save the transient consistency it would be necessary to keep, in such a scheme, $\Delta t/\Delta x^3$ very small; i.e., given $k < 1$, then

$$\Delta t = k\,\Delta x^3$$

or, in terms of α,

$$\alpha = k\,\Delta x. \tag{8}$$

This relation establishes, in practical applications, a very strict limit for α, much more than in the ordinary explicit scheme (if $\Delta x = 0.01$, $\alpha = O(\Delta x)$ instead of the classical $\alpha = 0.5$).

Furthermore, by setting $u^{(n+1)}$ to $u^{(n)}$ in (6) and by analysing the resulting truncation error, we note that consistency of the steady solution is not even guaranteed if (7) is disregarded.

4. NUMERICAL EXAMPLES

As claimed in [2, 4], the Richardson *et al.* discretization of the linear one-dimensional diffusion equation is unconditionally stable: the modulus of the amplification factor (obtained by means of the von Neumann stability analysis) is less than unity in the whole disturbance frequency range, for any value of the ratio α. Actually, as one can realize by looking at Fig. 1 (taken from the analysis in [4]), the amplification factor curves do not change any more when α is greater than about three.

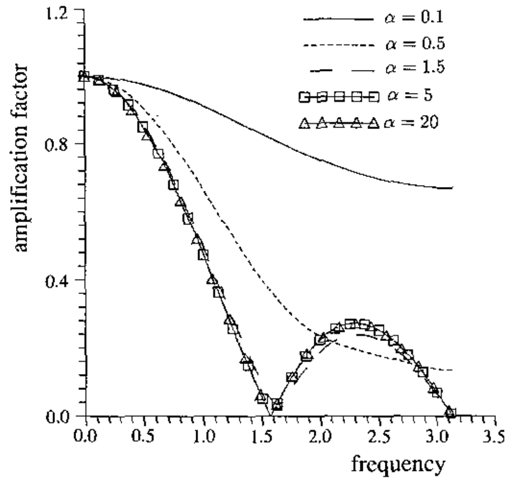

FIG. 1. Modulus of the amplification factor for the Richardson scheme.

On the other hand, when α reaches such high values the scheme suffers because of the inconsistency property shown in Section 3, so that the practical possibility of integrating the diffusion equation with arbitrarily high time steps was not found.

In Figs. 2 a–d we show some comparisons between the Richardson solution and the exact solution for the diffusion equation [5] with the usual homogeneous Dirichlet boundary conditions and $f(x) = \sin(\pi x)$ as the initial function; several values of the α parameter are tested with $\Delta x = 0.01$ and $x \in (0, 1)$. The solutions are presented after 50 iterations and show that, even for moderate value of α, the computed solution differs from the exact solution owing to a high-frequency disturbance and a slower decay rate for the low frequencies. Nevertheless, there is no way to get an instability for any frequency range.

5. CONCLUSIONS

We have analysed a scheme for the solution of finite difference equations recently proposed, placing special emphasis on the consistency analysis. The property of the scheme to be unconditionally stable has been verified for the simple one-dimensional diffusion model problem. This would be a very interesting feature for an explicit scheme making it extremely attractive for the solution of steady problems by means of a pseudo-transient iterative algorithm.

Nevertheless our analysis proved that, in order to ensure numerical consistency, a constraint on the time step even stronger than the stability limit of the classical explicit integration is required. This drawback has been confirmed by numerical experiments.

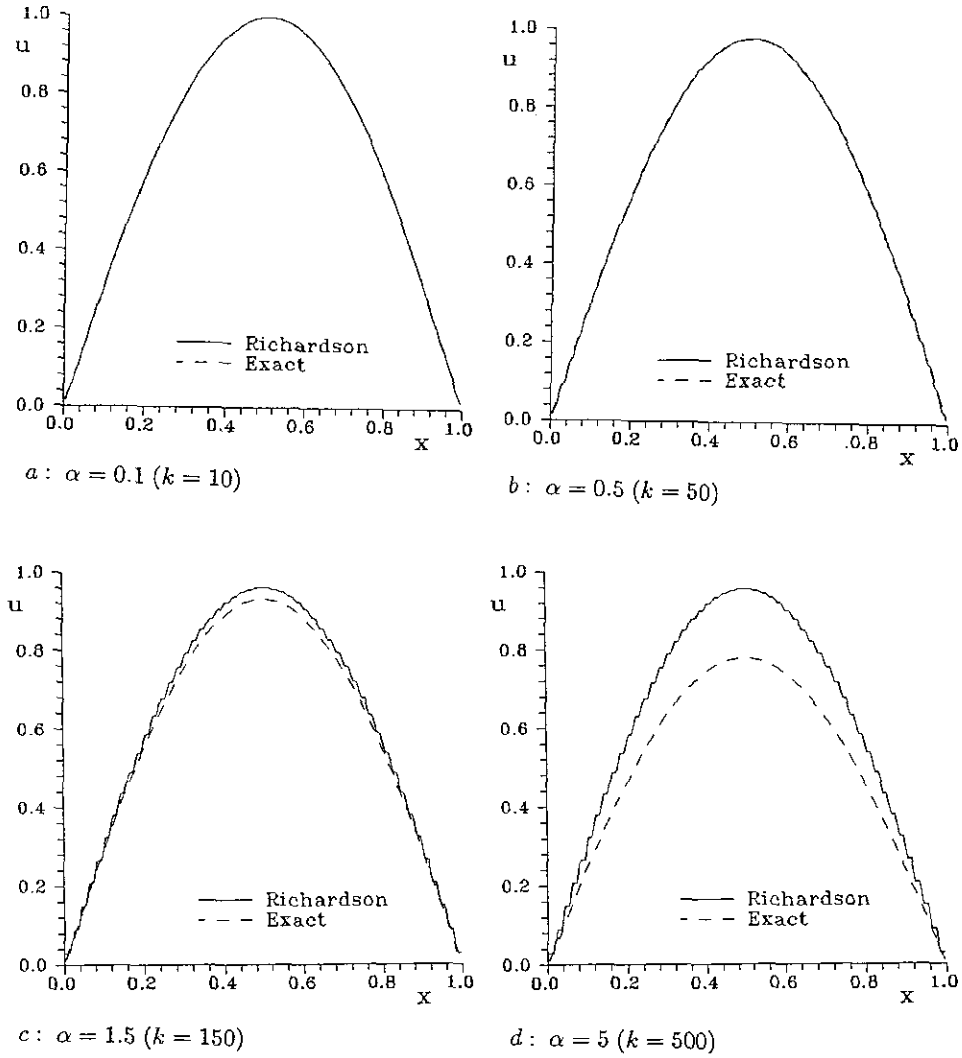

FIG. 2. Comparison between Richardson and exact solutions for the 1D diffusion model equation after 50 iterations ($\Delta x = 0.01$).

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