

Numerical Time-Stepping in Partial Differential Equations¹

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1. INTRODUCTION

The numerical solution of initial-value or initial boundary-value problems in partial differential equations (PDEs) has been studied for a considerable time already. Thanks to widely available computer facilities many important and interesting PDE problems from the engineering and physical sciences are nowadays solved by numerical methods. An outstanding field of applications is that of fluid dynamics, for example. In fact, computational fluid dynamics is still growing and seems to develop itself as an almost independent and self-supporting branch of science lying between mathematics and physics.

Due to the wide diversity in PDEs, there are many features which play a role in the construction and analysis of numerical methods: hyperbolic or parabolic character, number of space dimensions, nonlinearities, large gradients in the solution and discontinuities (shocks), shape of region, etc. In this note we will present a brief introduction to time-stepping schemes for time-dependent problems. Our aim is a presentation accessible to the non-specialist in numerical methods. We shall discuss the construction of some simple numerical time-stepping procedures and their stability. It should be emphasized that no part of the material presented here is new. In fact, the schemes and their properties we discuss have been known in the literature for a considerable time already. However, we also stress that these schemes, in spite of their simplicity, remain of continuing practical interest.

As a concrete example we shall use the linear *convection-diffusion equation*

1. Report of a lecture presented at the *General CWI-colloquium*

$$u_t + (v \cdot \nabla)u = \epsilon \Delta u, \quad t > 0, \quad x \in \Omega \subset \mathbb{R}^d, \quad (1.1)$$

where (scalar) $u(x, t)$ is the convected and diffused variable, $v = (v_1, \dots, v_d)^T$ is the convecting velocity vector (here constant), and $\epsilon > 0$ is a diffusivity parameter. We recall that ∇ is the gradient operator and Δ the Laplacian.

2. EXPLICIT AND IMPLICIT SCHEMES

For the time being we consider a general, linear time-dependent PDE of the form

$$u_t = Lu, \quad t > 0, \quad x \in \Omega \subset \mathbb{R}^d. \quad (2.1)$$

If we define the space-operator L by $Lu \equiv -(v \cdot \nabla)u + \epsilon \Delta u$, the convection-diffusion equation (1.1) is obtained. We will not specify boundary conditions for (2.1) as we do not discuss their influence here. The development of the time-stepping schemes will be carried through as if we were studying the initial-value problem.

Time-stepping schemes for the numerical integration of the evolution equation (2.1) are *step-by-step methods*. A step-by-step method proceeds from an approximation at $t = t_n$ one step of size τ to an approximation at $t = t_{n+1}$ where $t_{n+1} = t_n + \tau$. The choice of a scheme for (2.1) depends on various problem features as we mentioned in the introduction. A fundamental property of any scheme is that of stability. In this connection it makes sense to classify time-stepping schemes under three headings:

- a) explicit schemes;
- b) implicit schemes;
- c) explicit-implicit schemes;

which we shall use for the purpose of this presentation.

In the remainder of this section we shall discuss a simple example of an explicit and implicit scheme. Subsequently, in section 3 we shall present an interesting example of type c.

2.1. The explicit and implicit Euler scheme

To begin with, we shall discuss the *construction* of the forerunners of all integration schemes, viz., the *explicit* and *implicit Euler rule*. We note that the notions employed are of a much wider applicability. Let u be a solution of (2.1). Suppose that u is sufficiently differentiable and consider the Taylor expansion of $u(x, t_n + \tau)$ about t_n :

$$u(x, t_n + \tau) = u(x, t_n) + \tau u_t(x, t_n) + \frac{1}{2} \tau^2 u_{tt}(x, t_n) + \dots \quad (2.2)$$

When stepping from t_n to t_{n+1} any scheme tries to approximate, in some way or another, a truncated part of this series. Let us truncate after two terms:

$$u(x, t_n + \tau) \simeq u(x, t_n) + \tau u_t(x, t_n). \quad (2.3)$$

This is an approximate relation between exact solution values. By replacing this approximate relation by an exact one, but now between approximate solution values, a numerical scheme is obtained. This scheme is then said to be *consistent of order one* (in time) since (2.2) is approximated up to $O(\tau^2)$. The replacement itself determines the actual type of scheme.

Using the differential equation (2.1), (2.3) can be rewritten to

$$u(x, t_n + \tau) \simeq u(x, t_n) + \tau Lu(x, t_n). \quad (2.4)$$

We now define the approximation $U^n(x)$ for $u(x, t_n)$ by the exact relation

$$U^{n+1}(x) = U^n(x) + \tau LU^n(x), \quad (2.5)$$

which is the simplest of all integration schemes, viz., the *explicit Euler rule*. Note, however, that U^n is still space-continuous and L a space differential operator. To get a fully discrete approximation we next replace L by an appropriate *finite difference operator* L_h [1, 11, 13, 14, 15] so that (2.5) is replaced by

$$U_j^{n+1} = U_j^n + \tau L_h U_j^n. \quad (2.6)$$

The precise form of L_h is not of interest at the moment. Here we only note that U_j^n is a grid variable and approximates u at the space-time point (x_j, t_n) where x_j is a grid point from the finite difference grid Ω_h covering the space domain Ω . We observe that $L_h U_j^n$ is always a linear combination of grid values defined on a stencil around x_j . If the space dimension d is greater than 1, then j is a multi-index.

At each step with (2.6) an approximation error is made, the so-called *local discretization* or *truncation error*, which is accumulated during the stepping forward in time to the so-called *global discretization error*

$$\epsilon_j^n = u(x_j, t_n) - U_j^n. \quad (2.7)$$

The local error is found by recovering the truncated Taylor series (2.3) or (2.4) from (2.6). For this purpose we write down a perturbed version of (2.6), viz.,

$$\begin{aligned} u(x_j, t_{n+1}) &= u(x_j, t_n) + \tau L_h u(x_j, t_n) + \\ &\quad \tau(L - L_h)u(x_j, t_n) + \tau \rho(x_j, t_n) \\ &= u(x_j, t_n) + \tau u_t(x_j, t_n) + \tau \rho(x_j, t_n). \end{aligned} \quad (2.8)$$

Comparison with (2.2) shows that $\rho(x_j, t_n)$, which is the local error due to Euler's formula, satisfies

$$\rho(x_j, t_n) = \frac{1}{2} \tau u_{tt}(x_j, t_n) + O(\tau^2), \quad (2.9)$$

which once more reveals the first order consistency of Euler's rule. The quantity

$$\alpha(x_j, t_n) = (L - L_h)u(x_j, t_n) \quad (2.10)$$

is called the *space truncation error*. This error has nothing to do with the time-stepping scheme and originates from the replacement of L by L_h . If the grid Ω_h is refined, then $\alpha(x_j, t_n)$ should diminish accordingly. The (total) *local error* of the discretization (2.6) of (2.1) thus is given by

$$\beta(x_j, t_n) = \alpha(x_j, t_n) + \rho(x_j, t_n). \quad (2.11)$$

Finally, if we subtract (2.6) from its perturbed version (2.8), we get by definition of ϵ_j^n (2.7)

$$\epsilon_j^{n+1} = (1 + \tau L_h)\epsilon_j^n + \tau\beta(x_j, t_n). \quad (2.12)$$

The accumulation of the local errors $\beta(x_j, t_n)$, $0 \leq n \leq N-1$, to the global error ϵ_j^n at a fixed time $T = N\tau$, is described by this recursion. The *convergence question*, i.e., the question under which conditions on τ and h the global error ϵ^N at $t = T$ will decrease and how fast, obviously turns out to be a *stability question*. Loosely speaking, recursion (2.12) may be called *stable* if at each step the amplification of ϵ_j^n is not larger than by a factor $1 + O(\tau)$. Of course this depends on the metric used on the operator $1 + \tau L_h$, and thus on L_h and L . The interested reader is referred to [15] where the convergence question is extensively discussed. The notion of stability, in the sense of VON NEUMANN, will be taken up again in section 2.2.

The time-stepping scheme (2.6) is called the explicit Euler rule. A scheme is called explicit if the approximation at the new step point t_{n+1} is based only on previous approximations. The appellation *implicit* becomes clear if we slightly change (2.6) to the first order implicit Euler rule

$$U_j^{n+1} = U_j^n + \tau L_h U_j^{n+1}. \quad (2.13)$$

Here, U_j^{n+1} also appears in the right-hand side of the approximating equation which essentially requires the inversion of the operator $1 - \tau L_h$ at each time-step. In practice, this inversion implies the inversion of an associated, well-structured finite difference or finite element matrix [11, 12], which is carried out either by some form of Gaussian elimination or in an iterative fashion. For this reason one time step with (2.13) is more costly than one step with the explicit scheme (2.6), especially if $d > 1$. However, it still may be attractive to use (2.13), viz., if stability restricts the step size value τ in the explicit scheme. In virtually all applications the implicit Euler rule is stable for all $\tau > 0$ (unconditional stability [3]). In section 2.2 we shall illustrate this for the convection-diffusion equation (1.1). Finally, despite their low order of consistency, both Euler rules are frequently employed in numerical practice. This is particularly the case if problems are highly complicated as in computational fluid dynamics (see, e.g., [2] and [9] for an application of the implicit and explicit scheme, respectively).

2.2. Von Neumann stability

A central theme in the development and analysis of time-stepping schemes is that of *stability*. Consider again the explicit Euler rule and its error scheme (2.12). Stability there was taken to mean that, in some metric the amplification of ϵ_j^n to ϵ_j^{n+1} is not larger than by a factor $1 + O(\tau)$. In practice it is usual to insist on a stability condition which guarantees an *amplification factor not larger than 1*, since this best mimics the behaviour of the true solution of the problem, at least for the convection-diffusion equation (1.1). For constant coefficient problems, such as (1.1), most common is a *Fourier analysis* as proposed by VON NEUMANN (see [15]). Here we illustrate this analysis for equation (1.1).

Unless otherwise stated we let $d=1$, so we consider the one-dimensional problem

$$u_t + vu_x = \epsilon u_{xx}, \quad t > 0, \quad (2.14)$$

whereby we suppose that L_h is defined by second order *central finite differences*: $x_j = jh$ and [1, 11, 13, 15]

$$L_h U_j = \frac{\epsilon}{h^2}(U_{j+1} - 2U_j + U_{j-1}) - \frac{v}{2h}(U_{j+1} - U_{j-1}). \quad (2.15)$$

For the sake of brevity it is convenient to introduce the finite difference operators

$$\delta^2 U_j = U_{j+1} - 2U_j + U_{j-1}, \quad H U_j = (U_{j+1} - U_{j-1})/2. \quad (2.16)$$

Then the explicit Euler scheme (2.6) applied to (2.14) reads

$$U_j^{n+1} = \left(1 + \frac{\tau\epsilon}{h^2}\delta^2 - \frac{\tau v}{h}H\right)U_j^n. \quad (2.17)$$

Consider the convection-diffusion equation (2.14). Corresponding to the initial data $u(x,0) = \exp(i\omega x)$, $i^2 = -1$, $\omega \in \mathbb{R}$, the solution of (2.14) satisfies

$$u(x_j, t_n) = e^{-n(\tau\epsilon\omega^2 + i\tau v\omega)} e^{i\omega x_j}. \quad (2.18)$$

We see that the absolute value of the exponential is less than or equal to one for all $\epsilon \geq 0, v \in \mathbb{R}$, and any Fourier mode $\exp(i\omega x)$. The *Fourier (or von Neumann) stability method* applied to (2.17) now consists of examining Fourier modes

$$U_j^n = \xi^n e^{i\omega x_j}, \quad (2.19)$$

and deriving conditions on τ and h such that, in agreement with the behaviour of the exponential in (2.18) the (complex valued) amplification factor ξ satisfies

$$|\xi| \leq 1. \quad (2.20)$$

If (2.20) is true, the time-stepping scheme is called *stable in the (strict) sense of von Neumann*. The adjective *strict* refers to the fact that $|\xi| \leq 1$ rather than

$|\xi| \leq 1 + O(\tau)$ which is the original condition [15]. Hereafter we will omit this adjective. Obviously, for any method ξ approximates the exponential in (2.18). Here we do not discuss this further but concentrate on the stability question.

Some remarks are in order. Fourier analysis is based on the hypothesis that the problem and its approximating scheme admit solutions such as (2.18) and (2.19), respectively. Strictly speaking, Fourier analysis applies only to the problem with periodic boundary conditions or to the pure initial-value problem on the infinite x -axis. Also, it is required that the initial function possesses a Fourier series. Further, we take the wave number ω continuous in \mathbb{R} while the given mesh actually allows us to consider only a discrete set. Loosely speaking, the error made here is $O(h^2)$ and therefore we will follow precedent and let ω be continuous [15]. Despite these constraints, ‘the von Neumann method is generally the best single technique for analysing the stability of difference schemes. It should always be part of a stability analysis, even if other techniques are also employed’ (quotation from [9], p.890).

On substituting the Fourier mode (2.19) into the difference scheme (2.17), the value for $\xi = U_j^{n+1}/U_j^n$ is obtained. As a function of the phase angle $\theta = \omega h$ it is given by

$$\xi = 1 - \alpha(1 - \cos \theta) - ic \sin \theta, \quad (2.21)$$

where

$$\left\{ \begin{array}{l} \alpha = \frac{2\epsilon\tau}{h^2} \text{ (is called the diffusion parameter)} \\ c = \frac{v\tau}{h} \text{ (is called the Courant number)} \end{array} \right. \quad (2.22)$$

Here we have used the simple properties

$$\delta^2 e^{i\omega x_j} = 2(\cos \theta - 1)e^{i\omega x_j}, \quad He^{i\omega x_j} = i(\sin \theta)e^{i\omega x_j} \quad (2.23)$$

We are now ready to establish conditions on the diffusion parameter α and the Courant number c in order that the explicit Euler - central difference scheme (2.17) is stable in the sense of von Neumann. It can be shown that $|\xi| \leq 1$ for all θ if and only if

$$c^2 \leq \alpha \leq 1. \quad (2.24)$$

Hence this pair of inequalities is necessary and sufficient for stability in the sense of VON NEUMANN (see [9] and the reference therein) The diffusion barrier $\alpha \leq 1$ implies that

$$\tau \leq \frac{1}{2\epsilon} h^2. \quad (2.25)$$

which is a severe restriction on the time-step τ if ϵ is not small. Such a

restriction on τ is found for virtually all explicit methods and unacceptable for numerical practice. Inequality (2.25) is acceptable only if ϵ is small, hence if $|v| \gg \epsilon$ (dominating convection term). Unfortunately then the *convection-diffusion barrier* $c^2 \leq \alpha$, or

$$\tau \leq \frac{2\epsilon}{v^2}, \quad (2.26)$$

spoils the game. In fact, in the absence of diffusion ($\epsilon=0$) we always have instability illustrating that for the purely hyperbolic problem the explicit Euler - central difference scheme is of no use at all.

Similar negative results are found for the multi-dimensional problem (1.1). For full details we refer to the interesting and previously mentioned paper [9] by HINDMARSH, GRESHO and GRIFFITHS. They present a comprehensive study regarding the numerical stability of the simple explicit Euler formula combined with various spatial discretizations, including finite elements. In the next section we shall discuss an alternative scheme, nearly as simple as explicit Euler, which can be used with standard central differences and does not suffer from the convection diffusion barrier $c^2 \leq \alpha$.

To contrast the explicit Euler-finite difference scheme with its *implicit* counterpart (see (2.13))

$$U_j^{n+1} = U_j^n + \left(\frac{\tau\epsilon}{h^2} \delta^2 - \frac{\tau v}{h} H \right) U_j^{n+1}, \quad (2.27)$$

let us compute the amplification factor ξ for this implicit scheme. Using relations (2.22 and 2.23) we get

$$\xi = (1 + \alpha(1 - \cos \theta) + i c \sin \theta)^{-1}, \quad (2.28)$$

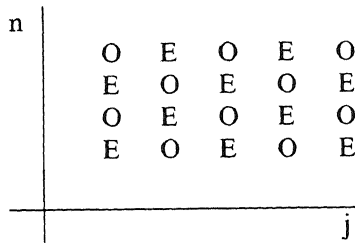
and an elementary calculation shows that $|\xi| \leq 1$, for all θ , for any nonnegative value of the diffusion parameter α and any value of the Courant number c . Consequently, stability limits such as (2.25) and (2.26) do not exist for the implicit Euler - finite difference scheme. The scheme is said to be *unconditionally stable*.

For numerical time-stepping purposes the property of unconditional stability is ideal in the sense that we then have the freedom to adjust the stepsize τ completely to the accuracy (in time) desired. Unfortunately, as we mentioned before, implicit steps may be rather expensive when compared with explicit steps, particularly so in two-dimensional and three-dimensional spaces. In practice, the choice of using explicit or implicit time-stepping is generally influenced by various factors, e.g., ease of programming (explicit schemes are invariably easier to apply than implicit ones) and computer facilities (available memory storage and central processor time). No doubt problems exist which must be treated implicitly just for the sake of numerical stability. In other cases, however, implicit time-stepping may be a bit superfluous and then appropriate explicit or explicit-implicit schemes can be quite useful.

3. AN EXPLICIT-IMPLICIT SCHEME

The appellation *explicit-implicit* refers to the fact that such schemes are based on a combination of explicit and implicit calculations. The objective of such a combination is always to reduce the computational effort of a fully implicit step to an acceptable level and in such a way that the resulting combination still offers attractive stability properties (in the literature one often uses the phrase *splitting* instead of explicit-implicit). Here we shall present an interesting example, viz., the *odd-even hopscotch* scheme which combines the explicit and implicit Euler rules (2.6) and (2.13). This combination was introduced by GORDON [4]. GOURLAY [5,6] has made a thorough study of Gordon's combination and has suggested various generalizations (see also [7], p.777 for more references).

Consider the explicit Euler - finite difference scheme (2.6) and its implicit counterpart (2.13). Let us suppose that the problem is one-dimensional (just for simplicity of presentation) and that L_h is a 3-point operator, i.e., $L_h U_j$ is a linear combination of U_{j-1}, U_j, U_{j+1} , for example the convection diffusion operator (2.15). Next consider the time-space mesh in the figure below



where the mesh points have been divided into two sets of points, viz., the points E where $(n+j)$ is even and the points O where $(n+j)$ is odd. GORDON's idea was now to use the explicit scheme at the odd points, for some fixed value of n , and then, for the same value of n , the implicit scheme at the even points:

$$U_j^{n+1} = U_j^n + \tau L_h U_j^n, \quad (n+j) \text{ odd}, \quad (3.1)$$

$$U_j^{n+1} = U_j^n + \tau L_h U_j^{n+1}, \quad (n+j) \text{ even}. \quad (3.2)$$

For example, for (2.15) this can be written as

$$U_j^{n+1} = U_j^n + \frac{\tau \epsilon}{h^2} (U_{j+1}^n - 2U_j^{n+1} + U_{j-1}^n) - \frac{\tau \nu}{2h} (U_{j+1}^n - U_{j-1}^n) \quad (3.1a)$$

$$U_j^{n+1} = U_j^n + \frac{\tau \epsilon}{h^2} (U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) - \frac{\tau \nu}{2h} (U_{j+1}^n - U_{j-1}^n) \quad (3.2a)$$

Because first all U_j^{n+1} , where $(n+1+j)$ is even, are computed, for a fixed n , it immediately follows that Gordon's scheme (3.1a) - (3.1b) is essentially explicit

and therefore easy to program. Note that at the following time step the roles of odd and even formulas are interchanged. GOURLAY has introduced the name hopscotch for this type of explicit-implicit scheme because of its progress through the time-space mesh.

As observed by GOURLAY the scheme (3.1) can be reformulated in terms of a single equation as follows:

$$U_j^{n+1} = U_j^n + \tau\theta_j^n L_h U_j^n + \tau\theta_j^{n+1} L_h U_j^{n+1}, \quad (3.3)$$

where $\theta_j^n = 1$ for $(n+j)$ odd and $\theta_j^n = 0$ for $(n+j)$ even. This formulation is useful as a starting point for the von Neumann stability analysis which we shall discuss now for the central difference operator (2.15).

Before we can apply the von Neumann stability analysis some preparatory work has to be done. First we write down the step from t_{n+1} to t_{n+2}

$$U_j^{n+2} = U_j^{n+1} + \tau\theta_j^{n+1} L_h U_j^{n+1} + \tau\theta_j^{n+2} L_h U_j^{n+2}, \quad (3.4)$$

and subtract (3.3) from (3.4):

$$U_j^{n+2} = 2U_j^{n+1} - U_j^n + \tau\theta_j^{n+2} L_h U_j^{n+2} - \tau\theta_j^n L_h U_j^n. \quad (3.5)$$

This equation takes a particularly simple form at the *even points* since there $\theta_j^n = \theta_j^{n+2} = 0$, viz.,

$$U_j^{n+2} = 2U_j^{n+1} - U_j^n, \quad (n+j) \text{ even.} \quad (3.6)$$

Note that this is a simple *three-level extrapolation* formula. To get a workable three-level formula for the odd points the expression for U_j^{n+1} from (3.3) is substituted into (3.4). Then, taking into account that for the odd points $\theta_j^{n+1} = 0$ and $\theta_j^n = \theta_j^{n+2} = 1$, we get

$$U_j^{n+2} = U_j^n + \tau L_h U_j^n + \tau L_h U_j^{n+2}, \quad (n+j) \text{ odd.} \quad (3.7)$$

Finally, by inserting (2.15) and the relation (3.6) for the even points, we arrive at the following *three-level scheme at the odd points*:

$$U_j^{n+2} = U_j^n + \frac{2\tau\epsilon}{h^2}(U_{j+1}^{n+1} - (U_j^{n+2} + U_j^n) + U_{j-1}^{n+1}) - \frac{\tau\nu}{h}(U_{j+1}^{n+1} - U_{j-1}^{n+1}), \quad (n+j) \text{ odd.} \quad (3.8)$$

If we ignore the start and the completion of the odd-even hopscotch process, we see that this process produces numerical solutions at the complete set of uncoupled odd points which satisfy the three-level scheme (3.8). This three-level scheme is known as the *leapfrog-Du Fort-Frankel scheme*. This equivalence is employed for the von Neumann stability analysis of the hopscotch scheme. Let us substitute the Fourier mode (2.19) into (3.8). We then find that the associated amplification factor ξ must be a root of the quadratic equation

$$(1 + \alpha)\xi^2 - 2(\alpha \cos \theta - i c \sin \theta)\xi - (1 - \alpha) = 0. \quad (3.9)$$

For von Neumann stability we thus want both roots of (3.9) on the unit disk for all θ . Using well-known results [8,10] this is the case if and only if the complex number

$$\lambda = 1 - (1 - \cos \theta) - i c \sin \theta \quad (3.10)$$

satisfies $|\lambda| \leq 1$ for all θ . We see that λ is of type (2.21) (with $\alpha = 1$) and we immediately conclude that scheme (3.8), and thus also the odd-even hopscotch - finite difference scheme (3.1) - (3.2) with L_h given by (2.15), is stable in the sense of von Neumann iff $\tau|v| \leq h$ or

$$c^2 \leq 1. \quad (3.11)$$

This is in marked contrast to the result (2.24) for the explicit Euler - central difference scheme. We see that by alternating the explicit and implicit Euler rules in the odd-even hopscotch way — a simple and essentially explicit process — we are rid of the convection-diffusion barrier $c^2 \leq \alpha$. Moreover, the diffusion parameter α is no longer present in the inequality (3.11).

As we noted above, the scheme (3.8) is unconditionally stable for the parabolic part of the problem. Unfortunately, concerning this part the scheme shows a deficiency with respect to accuracy. If we substitute u and let $\tau, h \rightarrow 0$, the scheme approaches

$$u_t + vu_x = \epsilon u_{xx} - \epsilon \frac{\tau^2}{h^2} u_{tt} + O(\tau^2) + O(h^2) + O(\epsilon \tau^4 / h^2). \quad (3.12)$$

This implies that for $\tau \rightarrow 0$, τ/h fixed and $\tau|v| \leq h$, the numerical solution approaches the solution of a wrong equation. It is plausible to expect that in practise this deficiency is not very serious as long as ϵu_{tt} does not take too large values. If it should lead to inaccuracies the most simple remedy is to reduce the time step a little. One could also conceive of eliminating the term $\epsilon \tau^2 h^{-2} u_{tt}$ by an extrapolation device [16]. Finally we want to remark that the hopscotch process can be equally well applied for all θ in two-dimensional and three-dimensional spaces. The only restriction is that L_h allows the odd-even uncoupling [5,6,16].

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