EXPLICIT APPROXIMATION METHODS

FOR

INITIAL-VALUE PROBLEMS

by

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PREFACE

Explicit difference approximations of parabolic initial boundary value problems are usually stable only if a difference grid with a limited time-step is used. By considering the one-dimensional diffusion equation as an example, it is shown in the following work that simple smoothing formulas can be constructed which, when applied to solutions computed with unstable explicit difference equations, result in stable approximations of the solution of the differential equation. Such computational procedures can be expressed as explicit difference analogues of the problem considered.

Conversely, explicit difference approximations, which need not be defined for all points of the difference grid but must be stable for the specific grid used, can be written as non-unique combinations of an explicit difference approximation, which need not be stable, and a smoothing formula. By appropriate choice of these explicit difference approximations and smoothing formulas this procedure will be defined for all grid points. This new technique thus has the advantage that explicit difference approximations with comparatively weak stability requirements and/or small truncation errors can be used in practice.

The properties are discussed of a number of explicit difference approximations which become practically usable through this technique. Among these approximations are methods which are stable for any choice of the difference grid. One of these has a considerably smaller truncation error than comparable methods available up to now. In the case of every difference equation discussed, a suitable smoothing formula is given which makes it possible to use the equation in practice.

Owing to the weaker stability conditions of a number of these approximation methods, the computational work necessary to obtain a solution in these cases is considerably less than that required when the standard explicit methods presently available are employed.

In conclusion, a brief discussion follows of the extension of the smoothing technique to more general parabolic equations, including more-dimensional problems.

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LIST OF CONTENTS

LIST OF ILLUSTRATIONS

INTRODUCTION

Par. 0.1 The numerical solution of initial boundary value problems

As is well known, the majority of partial differential equations cannot be solved analytically. Thus various methods have been proposed for obtaining approximate solutions of such equations. Among these methods, that of finite differences is the one most generally applicable; it consists in replacing the differential equation by an appropriate difference equation in an elementary, but not unique, way.

In such an approximation of an initial boundary value problem, three problems are encountered, viz. those of consistency, convergence and stability.

As the continuous problem is approximated by a discrete problem defined over a difference grid, the following requirement has to be met: if the mesh is refined, the discrete and continuous problems must become equivalent. In this case the difference equation is said to be consistent with the differential equation.

Consistency by itself does not, however, ensure that the solution of the difference equation converges to the solution of the differential equation as the mesh is refined. To ensure this, convergence conditions have to be specified.

The third problem which has to be considered, is the question of stability. Stability can be interpreted in many different ways, but is usually meant to indicate insensitivity to errors, for example round-off errors, introduced during the course of a computation. Various tools are available [3], [7], [9], [17], [20], [21] by means of which stability conditions can be deduced for the linear difference equations to be discussed. If these conditions are not satisfied, a small error introduced in one of the computed values will be magnified to such an extent that the computed solution becomes useless after only a few computation cycles.

The difference equations which can be used to approximate initial boundary value problems, can usually be divided into two classes, viz. implicit and explicit equations. The implicit equations have the advantage that in general they are stable for any choice of the difference grid used. On the other hand, from a computational point of view they are not as attractive as the explicit equations, as they give rise to a set of simultaneous equations at every cycle of the computation. Each of these sets of equations has to be solved before it is possible to continue with the next cycle of the computation. In contrast, the explicit equations have the advantage that they give the solution explicitly at the end of every computation cycle and are thus generally considered to be most suitable for the treatment of nonlinear problems. Most of these explicit equations, however, are stable only if certain, usually very restrictive, requirements are met by the difference grid used for their definition. These stability conditions are particularly restrictive in the case of parabolic equations.

These considerations have prompted a number of investigations whose object has been the construction of difference approximations which combine weaker stability conditions with a comparatively simple process of computation [4], [10], [18], [22], [23], [24]. This is also the aim of the present thesis. The smoothing technique described makes it possible in practice to use more general explicit difference approximations (see also [24]) with weaker stability conditions than the standard explicit methods available at present. This is achieved without excessively increased computational complexity; in fact, in many cases the amount of work necessary to obtain the solution is actually less than that required when the standard explicit methods are used.

Par. 0.2 Definitions

In the preceding paragraph mention was made of the fact that if a difference equation is to yield an approximate solution of an initial boundary value problem, such a difference equation has to be a consistent, convergent and stable approximation.

It was mentioned that the consistency conditions are those for which the difference equation is an approximation of the differential equation considered. In practice, consistency can easily be verified by making a Taylor-series expansion of every term in the difference equation, see for example [3], [7], [17], [20]. Subtraction of the differential equation then gives the so-called truncation error, which can generally be expressed as a function of the size of the mesh.

With regard to the question of convergence, all the problems discussed in the following chapters will be such that well-known results can be used to ensure the convergence of the approximate solution of the initial boundary value problem considered.

The problem that remains to be dealt with, is that of stability. In the literature many different definitions of stability are given. Here only two of the most widely accepted definitions will be used: that given by Forsythe and Wasow [7], which will be called F-W-stability, and that first given by John [12] and later used by Lax and Richtmyer [14], [20], which will be called J-stability.*

Various methods have been developed by which conditions can be determined which ensure the stability of a given difference equation. The most widely applicable of these methods are available for ensuring J-stability [20]. This is therefore the stability

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* In the literature J-stability is often referred to as L-R-stability.

definition used in most of the following work. In the case of the difference equations considered in chapter II, it was found, however, that by using a result given in [7] it is very easy to determine conditions under which F-W-stability will be obtained. Thus this stability definition will be used there.

In order to formulate the initial boundary value problem, let $[0,T]$ be a real interval, G a domain with boundary Γ in R_m, the m-dimensional Euclidean space, and S the cylinder $G \times [0,T]$. Consider the following differential equation

$$\frac{\partial u(x,t)}{\partial t} = L\, u(x,t) \qquad \ldots\ldots (0.1)$$

defined in S with L a linear differential operator with respect to $x_1, x_2, \ldots\ldots, x_m$. In (0.1) $u(x,t)$ is written instead of $u(x_1, x_2, \ldots\ldots, x_m, t)$, and this form will be used in the remainder of this paragraph.

In addition, assume that homogeneous boundary conditions

$$\ell_i\, u = 0, \quad i = 1,2,\ldots\ldots,s \qquad \ldots\ldots (0.2)$$

on Γ', the cylindrical surface of S, and initial conditions

$$u(x,0) = \varphi(x) \qquad \ldots\ldots (0.3)$$

on G, are prescribed.

The operators L and ℓ_i will be assumed linear and independent of t. It will also be assumed that the initial value problem is well-posed in the sense of Hadamard, see for example [7].

A rectangular grid, S_Δ, which will be called the difference grid, is now defined over S, the co-ordinates of the grid points being given by $(j\Delta x,\ k\Delta t)$, j and k non-negative integers, $0 \leq k\Delta t \leq T$, $\Delta x,\ \Delta t > 0$. As in the definition of (0.1) it is assumed that $m = 1$, as this simplifies the formulas and the extension to more dimensions is obvious. A relation will be assumed between Δx and Δt such that, if $\Delta t \to 0$, $\Delta x \to 0$ also.

The differential equation (0.1) can now be replaced by difference equations. In the following chapters only explicit difference equations, defined over the grid S_Δ, which can be written in the form

$$U_{j,k+1} = \sum_{q=0}^{n} \sum_{p=-m}^{m} b_{p,-q} \, U_{j+p,k-q} \qquad \text{.....(0.4)}$$

with m, n integers, $m \geq 1$, $n \geq 0$, will be considered. In this $U_{j,k} = U(j\Delta x, k\Delta t)$ is thus an approximation to $u(j\Delta x, k\Delta t) = u(x,t)$, the solution of (0.1) in the point with co-ordinates (x,t).

The boundary conditions are replaced by

$$\ell_{\Delta,i} \, U_{j,k} = 0, \quad i = 1,2,\ldots\ldots,s, \qquad \text{.....(0.5)}$$

i.e. $\ell_{\Delta,i}$ is an operator which transforms the boundary conditions prescribed on Γ' to the boundary grid points of S_Δ. The initial conditions are replaced by

$$U_{j,k} = \Phi_k(j\Delta x), \quad k = 0,1,\ldots\ldots,n. \qquad \text{.....(0.6)}$$

In order to give the stability definition of Forsythe and Wasow (for a full description of their reasoning see [7])assume that the solution of the difference equation, U_{j_0,k_0}, at the grid point $(j_0\Delta x,\ k_0\Delta t)$ is replaced by $U_{j_0,k_0} + \epsilon$, where ϵ will be called the error at $(j_0\Delta x,\ k_0\Delta t)$. In practice this may, for example, be the effect of a round-off error. If the step-by-step solution in the t direction is computed with the difference equation using $U_{j_0,k_0} + \epsilon$ without the introduction of new errors, and the values obtained at the subsequent grid points are indicated by $\tilde{U}_{j,k}$, then $\tilde{U}_{j,k} - U_{j,k}$ is called the departure of the solution caused by the error at $(j_0\Delta x,\ k_0\Delta t)$. If errors are committed at more than one point, which is normally the case in practice, the error caused by these errors at a subsequent point is called the cumulative departure. In linear problems the cumulative departure caused by two errors is the sum of the departures caused by each error separately.

The order of magnitude of the cumulative departure can be used as a natural measure of stability. By this is meant the order of magnitude of the maximum departure in a given domain with respect to the mesh size Δt and the maximum absolute error, δ (say), as both quantities tend to zero.

Definition 0.1

A procedure will be called F-W-stable if the cumulative departure tends to zero with the maximum absolute error, δ, and, as $\Delta t \to 0$, does not grow faster than some power of Δt^{-1}.

According to Forsythe and Wasow ([7], p. 32) this definition of stability is justified by the fact that in all problems which have been mathematically analyzed, the order of magnitude of the departure is either a low power, $\nu > 0$, of Δt^{-1} or else an exponential function of Δt^{-1}, so that there is a genuine gap between the nature of stable and unstable methods. For a particular class of problems this was proved by Kreiss [13]. Also note that in the above use is made of the maximum norm.

In [26] it is shown that, in the case of linear problems, a F-W-stable difference scheme is convergent when the truncation error is a certain power, μ, of Δt, where $\mu > \nu$.

In [14] Lax and Richtmyer developed a theory of stability and convergence of linear difference equations, using the concepts and methods of functional analysis. (See also [12], [20].)

Assume that the initial function of the linear initial boundary value problem to be solved belongs to some Banach space B of functions of x alone. The particular norm used need only be specified at a later stage. It cannot be expected that a solution of the differential equation problem will exist for every initial function in B. Thus some reasonably mild conditions must be imposed on the initial boundary value problem and the space B. These conditions will not be discussed in detail here. They amount essentially to requiring that the initial boundary value problem be well-posed and that every function of B can be approximated by initial functions for which a genuine solution ([20], p. 40) exists. These assumptions make it possible to associate with every initial function in B a solution in a somewhat generalized sense. For any fixed value of t such a solution is a function of x alone. This function will be an element in B, and it is a limit (in the norm of B) of genuine solutions of the differential equation.

The solutions, $U_{j,k}$, of the difference equations to be studied, are defined only at the points of a grid. If $U_{j,k}$ is to be an element of B for fixed t, its definition must be extended over the whole x interval under consideration. Assume that a method exists by which this can be accomplished, for example linear interpolation, and denote these values by U(x,t).

In the framework of these ideas, the solution U(x,t) of a difference problem will be said to converge to a solution u(x,t) of a differential problem if

$$\lim_{\Delta t \to 0} \| U(x,t) - u(x,t) \| \to 0.$$

A finite difference problem is called convergent if its solution converges to that of the formally corresponding initial boundary value problem for all initial functions in B.

<u>Definition 0.2</u>

A finite difference equation is called J-stable if the solution U(x,t) corresponding to an initial function $\varphi(x)$ satisfies a boundedness relation of the form

$$\|U(x,t)\| \leq M(t) \quad \|\varphi(x)\| \quad \text{for } 0 \leq t \leq T,$$

where $M(t)$ is independent of Δt. This relation is to be true for all $\varphi(x) \in B$.

If the terms convergence and stability are understood as just explained, it can be proved that, for a difference equation approximating a differential equation in the formal sense, stability is a necessary and sufficient condition for convergence. This result is known as Lax's equivalence theorem([20], p. 45).

Using the L_2 norm, a number of methods are deduced in [20] which can be applied to a wide class of problems to determine conditions under which stability will be obtained.

Par. 0.3 Summary of results given in the following chapters

As was mentioned in par. 0.1, most explicit difference equations are stable only if certain requirements are met by the difference grid used for their definition. If these stability conditions are not fulfilled, the computed solution departs exponentially from the analytic solution of the differential equation. It is well known that in the case of the one-dimensional heat equation, for example, such unstable approximate solutions computed with certain consistent explicit approximations oscillate with respect to the true solution [3], [17], [20]. This raises the question as to whether it is possible to construct smoothing formulas which, when applied to such an unstable solution, will give an approximate solution of the differential equation considered. That this is indeed possible, is shown in the following chapters.

These computational procedures can be expressed in terms of other explicit difference approximations of the initial boundary value problem considered. In fact, it is shown that a variety of combinations of unstable equations and smoothing formulas are equivalent to a single difference approximation.

Reversing this process leads to the result that explicit difference equations can be expressed in terms of combinations of smoothing formulas and other, often simpler, but not necessarily stable, difference equations. The main advantage of this is that a difference equation which, as a result of being defined over a large number of grid points on the next time-level, can be rewritten as a computational procedure which is defined for all these grid points. This procedure is not unique, but is equivalent to the original difference equation. This makes it possible to use more general explicit difference approximations with weaker stability conditions and smaller truncation errors to solve the initial boundary value problem considered. Other methods exist [24] which can be employed to enable difference equations, not defined for all grid points on the next time-level, to be applied to practical problems. All of these methods have disadvantages, especially with respect to extra errors introduced, which become more pronounced in the case of difference equations defined for relatively few grid points on the next time-level or which have comparatively small truncation errors.

The use of the smoothing technique involves two main disadvantages which are common to all the other above-mentioned methods. In the first place such a procedure involves more computational work than is necessary for obtaining a solution with the original difference equation. Thus the method is usually used to compute values only at those grid points for which the original difference equation is not defined. As difference equations with comparatively weak stability conditions can, however, be used in this way, the procedure often leads to an actual reduction in the total amount of computational work involved.

A second disadvantage of the method is that it does complicate programming to a certain degree.

In the following chapters various explicit difference approximations to simple one- and two-dimensional parabolic differential equations are discussed.

In chapter I a number of approximations to the one-dimensional diffusion equation are considered. Throughout this chapter, as well as in chapters III and IV, the stability definition 0.2 is used. In the relevant places, criteria are given which can be used to deduce the stability conditions.

Chapter II contains an extension of some of the results of chapter I. Here it was found more convenient, however, to use the stability definition 0.1.

In chapter III an approximation of a more general one-dimensional parabolic equation is given.

Finally, chapter IV contains a discussion of an example of the extension of the results of chapter I to two-dimensional problems.

CHAPTER I

EXPLICIT DIFFERENCE APPROXIMATIONS OF THE ONE-DIMENSIONAL DIFFUSION EQUATION, USING A SMOOTHING TECHNIQUE

Par. 1.1 The initial boundary value problem considered

As mentioned in the introduction, to solve the stability problem for approximating difference equations for parabolic differential equations is usually much more burdensome than for hyperbolic equations. Thus only linear parabolic equations will be considered in this chapter and the following ones. In order to simplify the deduced results, the differential equation as well as the boundary conditions will be assumed homogeneous and the coefficients of the differential equation constant. If need be, the obtained results can be extended to include the more general cases.

Consider the heat conduction equation

$$u_t = \sigma u_{xx},\ \sigma > 0,\ 0 < x < 1,\ 0 < t \leq T \quad \ldots\ldots (1.1)$$

with $u = u(x,t)$ and given initial and boundary conditions

$$u(x,0) = \varphi(x), \qquad 0 \leq x \leq 1,$$
$$u(0,t) = u(1,t) = 0, \qquad 0 < t \leq T. \qquad \ldots\ldots (1.2)$$

This problem is well-posed (see par. 0.2). For a detailed discussion of the properties of this equation and the available analytical solutions, the reader is referred to the extensive literature on the subject, e.g. [2].

Par. 1.2 An unstable explicit difference approximation

In order to obtain an approximate solution of the initial boundary value problem (1.1),(1.2), the differential equation may be replaced by a suitable difference equation.

For this purpose a rectangular difference grid is defined over the domain of definition of the differential equation. The mesh-width along the spatial co-ordinate axis is indicated by Δx

and that along the t-axis by Δt, with $\Delta x > 0$, $\Delta t > 0$. The co-ordinates of the grid points are given by $(j\Delta x, k\Delta t)$, j and k non-negative integers and such that $j = 0,1,\ldots,M$, $M\Delta x = 1$ and $k = 0,1,\ldots$.

Writing $U_{j,k} = U(j\Delta x, k\Delta t)$, the differential equation (1.1) can now be replaced by the difference equation

$$\frac{U_{j,k+1} - U_{j,k-1}}{2\Delta t} = \sigma \frac{U_{j-1,k} - 2U_{j,k} + U_{j+1,k}}{(\Delta x)^2} . \qquad \ldots\ldots (1.3)$$

This approximation was originally proposed by L.F. Richardson [19]. The initial and boundary conditions (1.2) are replaced by

$$\begin{aligned} U_{j,0} &= \Phi_j, \qquad j = 0,1,\ldots,M, \\ U_{0,k} &= U_{M,k} = 0, \qquad k = 0,1,\ldots . \end{aligned} \qquad \ldots\ldots (1.4)$$

It will always be assumed that the initial and boundary values can be computed to any desired degree of accuracy.

As the difference equation (1.3) is defined over three consecutive time-levels, values for $U_{j,k}$ on the time-levels $t = (k-1)\Delta t$ and $t = k\Delta t$ must be known in order to compute the solution on the time-level $t = (k+1)\Delta t$. Thus it will be assumed that a suitable approximation procedure is available with which the values $U_{j,1}$, $j=1,2,\ldots,M-1$, can be computed from the given initial and boundary values. Such an approximation is, for example, a difference approximation defined only over the two time-levels $t = (k-1)\Delta t$, $t = k\Delta t$.

The difference equation (1.3) is consistent with the differential equation (1.1). This can easily be established by making a Taylor-series expansion of the terms in (1.3) and subtracting (1.2) (see, for example, [20], p. 20). The difference is often called the truncation error, which in this case is given by

$$E = O((\Delta t)^2) + O((\Delta x)^2).$$

Various authors [3], [7], [17] have shown that the difference equation (1.3) is unstable for any choice of the difference grid. This can also be shown in the following way:

Assume that the initial values on the time-level $t = 0$ given by (1.4) are computed with round-off errors g_j, and the computed initial values on the time-level $t = \Delta t$ have errors h_j. These errors are propagated during a computation carried out with the difference equation (1.3). Thus the propagated error, $\epsilon_{j,k}$, must satisfy the following equations:

$$\epsilon_{j,k+1} = 2r\,\epsilon_{j-1,k} - 4r\,\epsilon_{j,k} + 2r\,\epsilon_{j+1,k} + \epsilon_{j,k-1}, \qquad \ldots\ldots (1.5)$$

$$\epsilon_{j,0} = g_j, \qquad \ldots\ldots (1.6)$$

$$\epsilon_{j,1} = h_j, \qquad \ldots\ldots (1.7)$$

$$\epsilon_{0,k} = \epsilon_{M,k} = 0, \qquad \ldots\ldots (1.8)$$

with $r = \sigma \dfrac{\Delta t}{(\Delta x)^2}$ assumed constant.

In order to construct an analytical solution of the difference equation (1.5), a product solution of the form

$$\epsilon^*_{j,k} = \gamma^k e^{ij\beta} \qquad \ldots\ldots (1.9)$$

is first sought.

By substituting this product into the difference equation, it follows that its real and imaginary parts will satisfy the equation if

$$\gamma^2 + (8r \sin^2 \frac{\beta}{2})\gamma - 1 = 0$$

i.e. if γ and β are related by

$$\gamma = -A \pm \sqrt{A^2+1} \qquad \ldots\ldots (1.10)$$

with

$$A = 4r \sin^2 \frac{\beta}{2}\,. \qquad \ldots\ldots (1.11)$$

To satisfy the conditions (1.8) the imaginary part $i\gamma^k \sin j\beta$ of (1.9) is chosen if β is real. This must be zero for $j = 0$ and $j = M$, i.e. the condition $\sin M\beta = 0$ must be imposed. Thus M-1 independent product solutions of the difference equation are obtained, each of the form $\gamma_\nu^k \sin j\beta_\nu$, $\nu = 1,2,\ldots\ldots,M-1$, with

$$\beta_\nu = \frac{\nu\pi}{M} . \qquad \ldots\ldots(1.12)$$

These solutions satisfy the boundary conditions (1.8) for any of the relations (1.10). By superposition the relation

$$\epsilon_{j,k} = \sum_{\nu=1}^{M-1} [a_\nu \gamma_1^k + b_\nu \gamma_2^k] \sin \frac{\nu j\pi}{M} , \qquad \ldots\ldots(1.13)$$

with

$$\gamma_1 = -A + \sqrt{A^2+1} ,$$

$$\gamma_2 = -A - \sqrt{A^2+1}$$

and now

$$A = 4r \sin^2 \frac{\nu\pi}{2M} ,$$

is deduced. This relation satisfies (1.5), (1.8) for arbitrary values of the constants a_ν, b_ν which are uniquely determined by the initial conditions (1.6) and (1.7). An explicit formula, involving finite sums of the g_j, h_j can easily be constructed [11].

As $\gamma_1 + \gamma_2 \leq 0$, $\gamma_1\gamma_2 = -1$ it follows that $\gamma_2 < -1$ for all ν between 1 and M-1. Thus those terms in (1.13) with γ_2 will grow exponentially, with alternating sign, for all $r > 0$ and increasing k, unless it happens that the corresponding coefficient a_ν, b_ν vanishes.

Such an exponential growth of the difference between the computed and analytical solutions has been observed in all solutions of the heat conduction equation (1.1) computed by use of the difference equation (1.3). The sign of the error alternates as k increases. (See Table I and the results given by O'Brien, Hyman and Kaplan [17]).

Par. 1.3 A smoothing formula

The question arises as to whether it is possible to construct a smoothing formula which, when applied to such an oscillating and exponentially increasing solution computed with the difference approximation (1.3), (1.4), will give a better approximation of the solution of the initial boundary value problem (1.1), (1.2).

Basically such an algorithm would consist of one or more computation cycles carried out using (1.3), (1.4) for $j = 1, 2, \ldots, M-1$. To these computed values of $U_{j,k}$, which will not, of course, be good approximations of the solution of the initial boundary value problem, a suitable smoothing formula is then applied. The problem is now to construct such a smoothing formula.

One obvious requirement of any such smoothing formula is, of course, that it should be relatively simple, i.e. its application should require as little computational work as possible. Apart from this, the algorithm has to be a consistent approximation of (1.1) and stable.

That it is indeed possible to construct such a smoothing formula can be shown for the following algorithm. Here it is assumed that a suitable approximation method is available with which values $U_{j,1}$ can be computed to any required degree of accuracy from the known values $U_{j,0}$, $j = 0, 1, \ldots, M$, given by (1.4).

Algorithm 1.1

Step 1: Using (1.3) the values $U_{j,2}$, $j = 1, 2, \ldots, M-1$, are computed from the known values $U_{0,1}$, $U_{M,1}$ and $U_{j,0}$, $j = 1, 2, \ldots, M-1$, given by (1.4) and the calculated values $U_{j,1}$, $j = 1, 2, \ldots, M-1$. This computation is then repeated to determine values $U_{j,3}$, $j = 1,2,\ldots\ldots,M-1$, using the known values $U_{j,1}$, $j = 1,2,\ldots\ldots,M-1$, and $U_{0,1}$, $U_{M,1}$, $U_{0,2}$, $U_{M,2}$ given by (1.4) as well as the calculated values $U_{j,2}$, $j = 1,2,\ldots\ldots,M-1$.

Step 2: To these known and computed values on the time-levels $t = 0$, $t = \Delta t$, $t = 2\Delta t$, $t = 3\Delta t$ a suitable smoothing formula is applied to give values $U'_{j,2}$, $j=1,2,\ldots\ldots,M-1$, on the time-level $t = 2\Delta t$, such that these values are good approximations to the solution of the differential equation.

Step 3: Using the known values on the time-level $t = \Delta t$ and the smoothed values on the time-level $t = 2\Delta t$, step 1 is repeated to give values for $t = 3\Delta t$, $t = 4\Delta t$. With these values step 2 is repeated to give smoothed values $U'_{j,3}$, $j = 1,2,\ldots\ldots,M-1$. This process can now be repeated for any desired number of cycles.

A smoothing formula such as is required in step 2 of this algorithm is given by theorem 1.2. In the proof of this theorem stability conditions have to be derived for a difference equation. In this derivation it has to be determined under which conditions all the roots of a given polynomial have negative real parts, i.e. whether the polynomial is of Hurwitz type. This can be deduced using the Routh-Hurwitz theorem [6], [8], [16], [25] of which Routh's formulation is given without proof by

<u>Theorem 1.1</u>

The equation

$$f(x) = a_0 x^n + a_1 x^{n-1} + \ldots\ldots + a_n = 0$$

with real coefficients a_ν, $\nu = 0,1,\ldots\ldots,n$, has exclusively roots with negative real parts if and only if the elements of the first column of the finite Routh scheme

$$\begin{array}{ccccc} a_0 & a_2 & a_4 & a_6 & \cdots\cdots \\ a_1 & a_3 & a_5 & a_7 & \cdots\cdots \\ \alpha_0 & \alpha_2 & \alpha_4 & \alpha_6 & \cdots\cdots \\ \beta_1 & \beta_3 & \beta_5 & \beta_7 & \cdots\cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{array}$$

with

$$\alpha_0 = \frac{a_1 a_2 - a_0 a_3}{a_1} \quad ,$$

$$\alpha_2 = \frac{a_1 a_4 - a_0 a_5}{a_1} \quad ,$$

$$\alpha_4 = \frac{a_1 a_6 - a_0 a_7}{a_1} \quad ,$$

$$\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot$$

$$\beta_1 = \frac{\alpha_0 a_3 - a_1 \alpha_2}{\alpha_0} \quad ,$$

$$\beta_3 = \frac{\alpha_0 a_5 - a_1 \alpha_4}{\alpha_0} \quad ,$$

$$\beta_5 = \frac{\alpha_0 a_7 - a_1 \alpha_6}{\alpha_0} \quad ,$$

$$\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot$$

are all non-zero and have the same sign.

In many cases Hurwitz's formulation is preferred, but in the following applications the use of the Routh scheme is somewhat more convenient.

For the treatment of singular cases, see, for example, [8].

<u>Theorem 1.2</u>

Given an approximate solution of the initial boundary value problem (1.1), (1.2) for the time-levels $t = (k-1)\Delta t$, $t = k\Delta t$ and values for the time-levels $t = (k+1)\Delta t$, $t = (k+2)\Delta t$ computed according to step 1 of algorithm 1.1, then the smoothing formula

$$U'_{j,k+1} = \sum_{\ell=-1}^{2} a_\ell \, U_{j,k+\ell}, \quad j = 1,2,\ldots,M-1, \qquad \ldots\ldots(1.14)$$

$$k = 1,2,\ldots$$

with

$$a_0 = 1 - a_2,$$

$$a_1 = -a_{-1} = \frac{1}{2} - a_2 \qquad \ldots\ldots(1.15)$$

and with a_2 such that (Fig.1)

(i) for $0 < r \leq \dfrac{\sqrt{6}-2}{4(5-2\sqrt{6})}$ ($\approx 1\cdot112\ 372$):

$$\frac{2r-1}{8r(4r+1)} \leq a_2 \leq \frac{1}{16r}$$

and

(ii) for $\dfrac{\sqrt{6}-2}{4(5-2\sqrt{6})} \leq r \leq \dfrac{1}{4(5-2\sqrt{6})}$ ($\approx 2.474\ 745$):

$$\frac{5-2\sqrt{6}}{4} \leq a_2 \leq \frac{1}{16r}, \qquad \ldots\ldots(1.16)$$

applied to these given values according to step 2 of algorithm 1.1, results in a consistent and stable approximation of (1.1), (1.2) with a truncation error given by

$$E = O(\Delta t) + O((\Delta x)^2). \qquad \ldots\ldots(1.17)$$

Proof:

The values $U_{j,k+2}$ and $U_{j,k+1}$, calculated by use of (1.3), can be expressed in terms of the given values $U_{j,k}$ and $U_{j,k-1}$ by use of (1.3), i.e. substitution of (1.3) into the right-hand side of (1.14) yields

$$U'_{j,k+1} = \sum_{q=0}^{1} \sum_{p=-2}^{2} b_{p,-q} \, U_{j+p,k-q} \qquad \ldots\ldots(1.18)$$

with

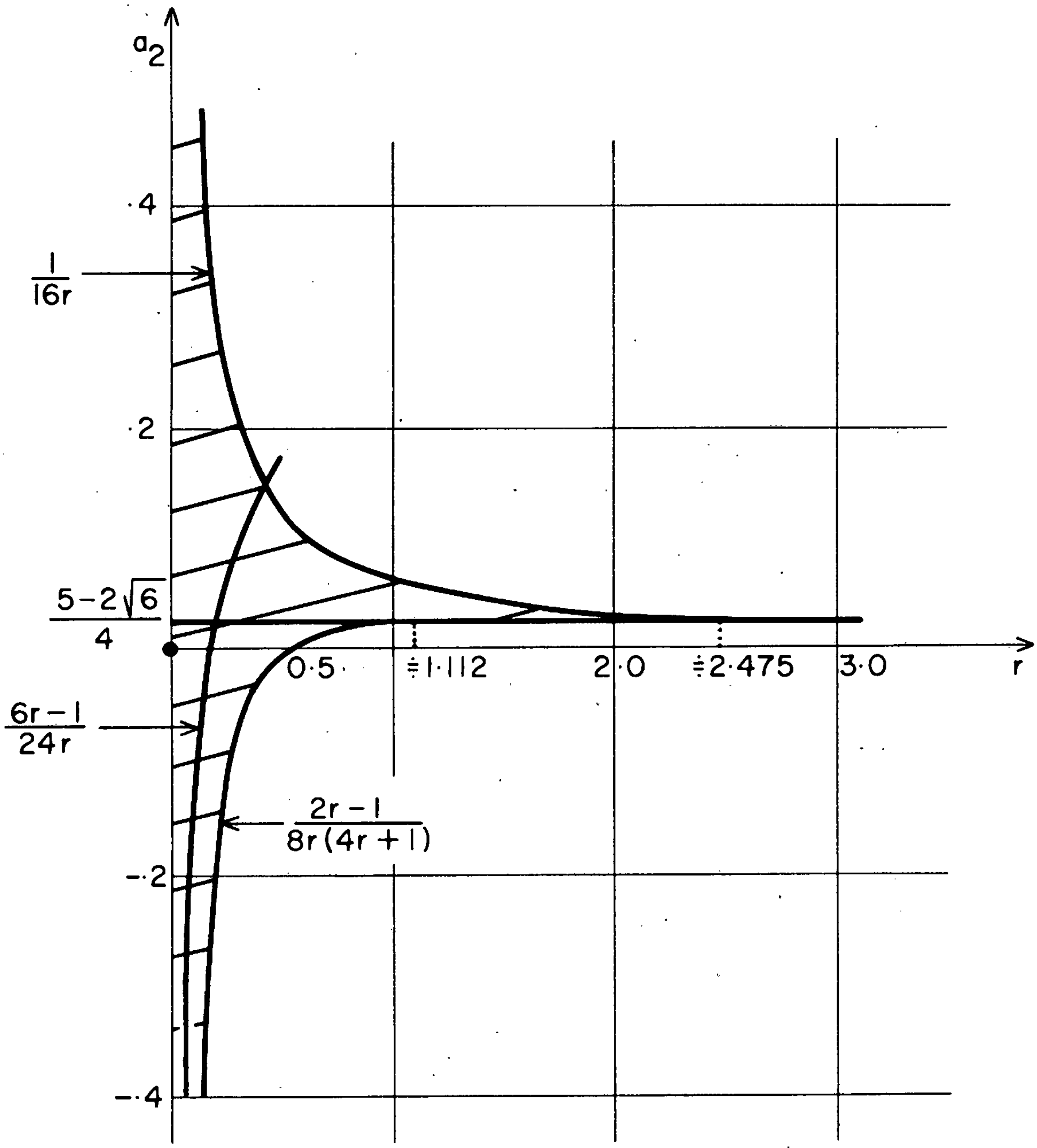

FIGURE I

XG4-1032

$$
\begin{aligned}
b_{0,0} &= a_0 - 4ra_1 + (1+24r^2)\, a_2 \\
b_{1,0} = b_{-1,0} &= 2ra_1 - 16r^2\, a_2 \\
b_{2,0} = b_{-2,0} &= 4r^2\, a_2 \\
b_{0,-1} &= a_{-1} + a_1 - 4r\, a_2 \\
b_{1,-1} = b_{-1,-1} &= 2r\, a_2 \\
b_{2,-1} = b_{-2,-1} &= 0. \qquad .....(1.19)
\end{aligned}
$$

Thus (1.18) is a difference equation which is equivalent to the algorithm given in the theorem, i.e. in order to prove the theorem it is necessary and sufficient to prove that (1.18) is a consistent and stable approximation of (1.1).

Using a Taylor-series expansion in the usual way [3], [17], [20] it can easily be shown that if the conditions (1.15) are satisfied, (1.18) will be a consistent approximation of (1.1), under the assumption that $r = \sigma \dfrac{\Delta t}{(\Delta x)^2}$ remains constant as $\Delta t \to 0$.

The truncation error is given by

$$E = O(\Delta t) + O((\Delta x)^2).$$

Using the definition of the amplification matrix in [20] and writing the two-level system of difference equations equivalent to (1.18):

$$
\begin{aligned}
U_{j,k+1} &= \sum_{p=-2}^{2} b_{p,0}\, U_{j+p,k} + \sum_{p=-2}^{2} b_{p,-1}\, V_{j+p,k} \\
V_{j+p,k+1} &= U_{j+p,k}\ , \quad p = 0, \pm 1, \pm 2 \qquad .....(1.20)
\end{aligned}
$$

the amplification matrix is

$$
G(\Delta t, \beta) = \begin{bmatrix} \sum_p b_{p,0}\, e^{ip\beta\Delta x} & \sum_p b_{p,-1}\, e^{ip\beta\Delta x} \\ 1 & 0 \end{bmatrix} \qquad .....(1.21)
$$

of which the characteristic equation is

$$\lambda^2 - S_0\lambda - S_{-1} = 0 \qquad .....(1.22)$$

with

$$S_0 = \sum_p b_{p,0} e^{ip\beta\Delta x} ,$$
$$S_{-1} = \sum_p b_{p,-1} e^{ip\beta\Delta x} . \qquad .....(1.23)$$

According to [20], see also [21], a necessary condition for the stability of (1.18) according to definition 0.2 is that for one eigenvalue of (1.21), say $\lambda^{(1)}$, the inequality

$$|\lambda^{(1)}| \leq 1 + O(\Delta t) \qquad .....(1.24)$$

must hold, whereas a sufficient condition is that for the remaining eigenvalues the condition

$$|\lambda^{(i)}| \leq \gamma < 1, \quad i = 2,3,..... \qquad .....(1.25)$$

must hold.

To deduce conditions that have to be fulfilled by the coefficients $b_{p,-q}$ of (1.18) in order that the inequalities (1.24), (1.25) may hold, one of the easiest methods is to make the transformation

$$\lambda = \frac{1+z}{1-z} , \qquad .....(1.26)$$

which maps the unit disk into the left half-plane, and then to apply theorem 1.1 to the transformed polynomial (1.22):

$$(1+S_0-S_{-1})z^2 + 2(1+S_{-1})z + (1-S_0-S_{-1}) = 0. \qquad .....(1.27)$$

By using the result given in theorem 1.1, conditions can be determined under which (1.27) will be a Hurwitz-polynomial. Use is made of the relations (1.15) and (1.19) in this lengthy, but elementary calculation. In the application of the Routh scheme in this case, some of the terms in the first column of the scheme can become zero. As was mentioned before, methods exist by which these singular cases can be treated. However, it is much easier to treat these by referring to the original characteristic equation (1.22). To sum up: application of the result of theorem 1.1

gives the condition (1.16), in which the equalities are ascertained by considering the characteristic equation directly.

This concludes the proof.

In the application of the algorithm 1.1 with the smoothing formula (1.18) near the boundaries, the values $U_{0,k+1}$ and $U_{M,k+1}$ are defined by the boundary conditions (1.4) rather than computed using (1.3). Previously it was assumed that the initial and boundary conditions could be computed to any desired degree of accuracy. Thus it may be assumed that the values $U_{0,k+1}$ and $U_{M,k+1}$ have been more accurately determined than they would have been if computed with (1.3).

In order to gain more insight into the effect of such an error, consider the case when, for example, $U_{j_1-1,k+1}$ is replaced by a more accurate value, j_1 being a specific value of j.

Putting

$$\epsilon_{j,k} = U_{j,k} - u(j\Delta x, k\Delta t)$$

the error made in the computation of $U_{j_1,k+2}$ using (1.3) is given by

$$\epsilon_{j_1,k+2} = 2r(\epsilon_{j_1+1,k+1} - 2\epsilon_{j_1,k+1} + \epsilon_{j_1-1,k+1}) + \epsilon_{j_1,k}$$

and

$$|\epsilon_{j_1,k+2}| \leq |\epsilon_1| + 2r|\epsilon_{j_1-1,k+1}|$$

with

$$\epsilon_1 = \epsilon_{j_1,k} + 2r(\epsilon_{j_1+1,k+1} - 2\epsilon_{j_1,k+1}) .$$

Now assume that $U_{j_1-1,k+1}$ is replaced by a more accurate approximation $\hat{U}_{j_1-1,k+1}$ of the solution of the differential equation. Thus, if

$$\hat{\epsilon}_{j_1-1,k+1} = \hat{U}_{j_1-1,k+1} - u((j_1-1)\Delta x, (k+1)\Delta t),$$

then

$$|\hat{\epsilon}_{j_1-1,k+1}| \leq |\epsilon_{j_1-1,k+1}| .$$

The value $\hat{U}_{j_1,k+2}$, computed with (1.3) using this more accurate value, thus has an error

$$\hat{\epsilon}_{j_1,k+2} = \epsilon_1 + 2r\,\hat{\epsilon}_{j_1-1,k+1}$$

and

$$|\hat{\epsilon}_{j_1,k+2}| \leq |\epsilon_1| + 2r|\hat{\epsilon}_{j_1-1,k+1}|$$
$$\leq |\epsilon_1| + 2r|\epsilon_{j_1-1,k+1}| .$$

Using the above notation, the error given by the smoothing formula (1.14) is

$$\epsilon'_{j_1,k+1} = a_{-1}\,\epsilon_{j_1,k+1} + a_0\,\epsilon_{j_1,k} + a_1\,\epsilon_{j_1,k+1} + a_2\,\epsilon_{j_1,k+2}$$

and

$$|\epsilon'_{j_1,k+1}| \leq |\epsilon_2| + |a_2|\,|\epsilon_{j_1,k+2}|$$
$$\leq |\epsilon_2| + |a_2|\,(|\epsilon_1| + 2r|\epsilon_{j_1-1,k+1}|) \qquad \ldots\ldots (1.28)$$

with

$$\epsilon_2 = a_{-1}\,\epsilon_{j_1,k+1} + a_0\,\epsilon_{j_1,k} + a_1\,\epsilon_{j_1,k+1} .$$

In the same way, for the error given by the smoothing formula if $\hat{U}_{j_1-1,k+1}$ is used instead of $U_{j_1-1,k+1}$, the following holds

$$|\epsilon'_{j_1,k+1}| \leq |\epsilon_2| + |a_2|\,|\hat{\epsilon}_{j_1,k+2}|$$
$$\leq |\epsilon_2| + |a_2|\,(|\epsilon_1| + 2r|\hat{\epsilon}_{j_1-1,k+1}|). \qquad \ldots\ldots (1.29)$$

Similar results can be deduced if $U_{j_1+1,k+1}$ is replaced by a more accurate approximation.

The results (1.28) and (1.29) are substantiated by results obtained in practical computations (see, for example, Table I, columns 4 and 5; Table II, columns 3 and 4), i.e. the use of prescribed boundary values instead of values computed by use of (1.3) in step 1 of algorithm 1.1 does not adversely influence the accuracy of the results obtained.

According to the stability conditions (1.16) of theorem 1.2 stability can be obtained for all r such that *

$$0 < r \leq \frac{1}{4(5-2\sqrt{6})} \; (\approx 2.474\ 745). \qquad .....(1.30)$$

It is clear that the amount of work required to carry out a computation with the method of theorem 1.2 will be greater than that needed for the equivalent difference equation (1.18). On the other hand the method of theorem 1.2 is defined for all the grid points on the time-level $t = (k+1)\Delta t$, whereas (1.18) is not. Thus, in order to keep the amount of work involved to a minimum, the values $U_{1,k+1}$ and $U_{M-1,k+1}$ can be computed using the method of theorem 1.2. The remaining $U_{j,k+1}$, $j = 2,3,\ldots\ldots,M-2$, can then be computed with (1.18).

A question which arises, is what influence the choice of a_2 has on the approximation error. In order to get an indication of this, the fact can be used that the solution of the differential equation (1.1) also solves the equation $u_{tt} = \sigma^2 u_{xxxx} = \sigma u_{xxt}$ [7], [20] under the assumption that u is sufficiently smooth. Using these relations in a Taylor-series expansion of the difference equation (1.18) it follows that the truncation error will be

$$E = O((\Delta t)^2) + O((\Delta x)^4) \qquad .....(1.31)$$

if

$$a_2 = \frac{6r - 1}{24r} \; . \qquad .....(1.32)$$

---

* In Par. 1.7 it will be shown that a different choice of the smoothing formula will give a stable procedure for all

$0 < r < \frac{3+2\sqrt{2}}{2}$ ($\approx 2.914\ 214$). (See Table III, c.)

This condition for the choice of a_2 has to be fulfilled in addition to the conditions stated in theorem 1.2.

The assumptions of theorem 1.2 and (1.32) can be satisfied simultaneously only if (see Fig. 1)

$$0 < r \leq \frac{5}{12} . \qquad .....(1.33)$$

A numerical example:

Table I gives results computed using the above procedure. The problem considered is the heat equation (1.1) with $\sigma = 1$ and the same x- and t-intervals. The boundary conditions are the same as those given in (1.2). The initial condition is

$$u(x,0) = 4x(1-x), \qquad 0 \leq x \leq 1.$$

All the results in Table I give the computed change in temperature for increasing t at x = 0.5. In all computations Δx was kept fixed at 0.1, i.e. M = 10. Thus changes in r are only effected by changes in Δt.

The second column of the Table gives the analytical solution of the problem considered, [15].

The fourth column gives an approximate solution computed with the ordinary explicit difference approximation to (1.1):

$$U_{j,k+1} = (1-2r)U_{j,k} + r(U_{j-1,k} + U_{j+1,k}) \qquad .....(1.34)$$

with $r = \frac{1}{6}$. The truncation error of this equation is given by

$$E = O((\Delta t)^2) + O((\Delta x)^4)$$

[7], [20]. For reference purposes results computed with (1.34) with $r = \frac{1}{2}$ are given in the sixth column.

The remaining columns give approximate solutions computed with the procedure of theorem 1.2 for various values of r. In the case of r = 0.4 the condition (1.32) is satisfied. For r = 0.5 and larger values of r, the increase in the approximation error is noticeable.

TABLE I

t	Analytical solution	Approx. solution using (1.3) $r = 1.0$ $E=0((\Delta t)^2)+0((\Delta x)^2)$	Approx. solution using (1.34) $r = \frac{1}{6}$ $E=0((\Delta t)^2)+0((\Delta x)^4)$	Approx. solution using algorithm 1.1 and (1.14) $r = 0.4$ $a_{-1}=-0.354\ 167$ $a_0 = 0.854\ 167$ $a_1 = 0.354\ 167$ $a_2 = 0.145\ 833$ $E=0((\Delta t)^2)+0((\Delta x)^4)$	Approx. solution using (1.34) $r = 0.5$ $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using algorithm 1.1 and (1.14) $r = 0.5$ $a_{-1}=-0.375$ $a_0 = 0.875$ $a_1 = 0.375$ $a_2 = 0.125$ $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using algorithm 1.1 and (1.14) $r = 1.0$ $a_{-1}=-0.437\ 5$ $a_0 = 0.937\ 5$ $a_1 = 0.437\ 5$ $a_2 = 0.062\ 5$ $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using algorithm 1.1 and (1.14) $r = 1.5$ $a_{-1}=-0.458\ 333$ $a_0 = 0.958\ 333$ $a_1 = 0.458\ 333$ $a_2 = 0.041\ 666\ 7$ $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using algorithm 1.1 and (1.14) $r = 2.0$ $a_{-1}=-0.468\ 75$ $a_0 = 0.968\ 75$ $a_1 = 0.468\ 75$ $a_2 = 0.031\ 25$ $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (1.34) $r = 1.0$
0.00	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000
0.01	.919 331	.919 331	.920 003		.920 000	.920 005	.920 012			.920 000
0.02	.840 708	.842 868	.840 743	.840 789	.840 000	.840 738	.840 361		.840 885	.840 000
0.03	.764 897	.746 811	.764 873		.762 500	.764 352	.762 807	.762 036		.760 000
0.04	.694 326	.816 488	.694 301	.694 252	.690 625	.693 220	.689 511		.687 320	.680 000
0.05	.629 614	-.157 909	.629 592		.625 000	.628 211	.622 194			.600 000
0.06	.570 664	6.163 548	.570 646	.570 548	.565 430	.569 114	.561 598	.555 283	.551 656	.680 000
0.07	.517 124		.517 108		.511 475	.515 480	.507 280			-.040 000
0.08	.468 561		.468 548	.468 416	.462 646	.466 859	.458 335		.442 163	2.440 000
0.09	.424 540		.424 530		.418 472	.422 810	.414 048	.405 550		-6.280 000
0.10	.384 647		.384 639	.384 501	.378 513	.382 914	.373 972		.357 787	
0.11	.348 500		.348 493		.342 369	.346 779	.337 763			
0.12	.315 749		.315 742	.315 609	.309 676	.314 053	.305 072	.296 415	.288 578	
0.13	.286 074		.286 069		.280 105	.284 415	.275 557			
0.14	.259 189		.259 185	.259 059	.253 357	.257 572	.248 898		.232 387	
0.15	.234 830		.234 826		.229 164	.233 263	.224 815	.216 523		
0.16	.212 760		.212 757	.212 641	.207 280	.211 247	.203 058		.187 405	
0.17	.192 764		.192 762		.187 487	.191 309	.183 405			
0.18	.174 648		.174 647	.174 540	.169 583	.173 252	.165 654	.158 215	.151 069	
0.19	.158 234		.158 233		.153 390	.156 900	.149 620			
0.20	.143 363		.143 362	.143 266	.138 742	.142 090	.135 138		.121 834	

The amount of work needed to carry out one cycle of the computation using (1.34) with $r = \frac{1}{6}$ is of the same order of magnitude as that needed by the method of theorem 1.2 for $r = 0.4$, Δx being the same in both instances.

Par. 1.4 <u>The explicit difference equations to be considered</u>

In this and the subsequent paragraphs, also in the remaining chapters, it will be convenient to use the following definition:

<u>Definition 1.1</u>

A difference equation which is consistent with a differential equation and combines with a smoothing formula to give a computational procedure equivalent to another difference equation which approximates the same differential equation, will be called a basic difference equation.

From practical considerations it is of course clear that the basic difference equation should preferably not include more than three consecutive grid points along a spatial co-ordinate axis. The same requirement holds for any smoothing formula used. This ensures that these formulas are defined for all interior grid points.

In the rest of this chapter some of the properties will be discussed of explicit difference equations which approximate (1.1) and can be written as

$$b_{0,+1} U_{j,k+1} = \sum_{q=0}^{n} \sum_{p=-m}^{m} b_{p,-q} U_{j+p,k-q}$$

or, in normalized form

$$U_{j,k+1} = \sum_{q=0}^{n} \sum_{p=-m}^{m} \left(\frac{b_{p,-q}}{b_{0,+1}}\right) U_{j+p,k-q}, \qquad \ldots\ldots(1.35)$$

with $m \geq 1$, $n \geq 0$ integers. The coefficients in (1.35) will be used as they stand, as this facilitates the deduction of stability conditions in those cases when the time-derivative in the differential equation (1.1) is not approximated by using forward differences (see par. 1.8). It will again be assumed that the initial and boundary conditions (1.2) are replaced by suitable difference initial and boundary conditions, as for example in (1.4).

The main aim of this discussion will be to indicate some of the characteristics of the equations (1.35) as these become available for practical use through the smoothing technique described in par. 1.3, and not so much to give a detailed analysis of these approximations; for such an analysis the reader is referred, inter alia, to [3], [7], [9], [20], [21] and [24].

Using a Taylor-series expansion, as before, it can easily be shown that the above difference equation will be a consistent approximation of (1.1) if, with $\Delta t \to 0$

$$\begin{aligned} \sum_q \sum_p b_{p,-q} &= b_{0,+1} \\ \sum_q \sum_p q b_{p,-q} &= 1 - b_{0,+1} \qquad \qquad .....(1.36) \\ \sum_q \sum_p p^2 b_{p,-q} &= 2r \end{aligned}$$

with $r = \sigma \dfrac{\Delta t}{(\Delta x)^2}$ = const. and where the $b_{p,-q}$ are in general also functions of Δt.

As in the case of (1.20) and (1.21), the amplification matrix of this multi-level difference equation can be determined by writing the equivalent system of two-level equations:

$$U_{j,k+1} = \sum_p \frac{b_{p,0}}{b_{0,+1}} U_{j+p,k} + \sum_p \frac{b_{p,-1}}{b_{0,+1}} V^{(1)}_{j+p,k} + \sum_p \frac{b_{p,-2}}{b_{0,+1}} V^{(2)}_{j+p,k}$$

$$+ \cdot \cdot \cdot \cdot \cdot + \sum_p \frac{b_{p,-n}}{b_{0,+1}} V^{(n)}_{j+p,k} \quad ,$$

$$V^{(1)}_{j+p,k+1} = U_{j+p,k} \quad , \qquad p = 0, \pm 1, \ldots\ldots, \pm m,$$

$$V^{(2)}_{j+p,k+1} = V^{(1)}_{j+p,k} \quad ,$$

$$\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot$$

$$V^{(n)}_{j+p,k+1} = V^{(n-1)}_{j+p,k} \quad . \qquad \ldots\ldots(1.37)$$

The amplification matrix is now

$$G = \begin{bmatrix} \sum_p c_p \frac{b_{p,0}}{b_{0,+1}} & \sum_p c_p \frac{b_{p,-1}}{b_{0,+1}} & \sum_p c_p \frac{b_{p,-2}}{b_{0,+1}} & \cdots\cdots & \sum_p c_p \frac{b_{p,-n}}{b_{0,+1}} \\ 1 & 0 & 0 & \cdots\cdots & 0 \\ 0 & 1 & 0 & \cdots\cdots & 0 \\ 0 & 0 & 1 & \cdots\cdots & 0 \\ \cdot & \cdot & \cdot & \cdots\cdots & \cdot \\ 0 & 0 & 0 & \cdots\cdots & 0 \end{bmatrix} \qquad \ldots(1.38)$$

with

$$c_p = e^{ip\beta\Delta x} \quad , \qquad p = 0, \pm 1, \pm 2, \ldots\ldots, \pm m. \qquad \ldots\ldots(1.39)$$

The characteristic polynomial of G is

$$f(\lambda) = (-1)^{n+1} \lambda^{n+1} + (-1)^n \sum_{\ell=0}^{n} d_\ell \lambda^{n-\ell} \qquad \ldots\ldots(1.40)$$

with the

$$d_\ell = \frac{1}{b_{0,+1}} \sum_p c_p b_{p,-\ell}, \quad \ell = 0,1,\ldots\ldots,n. \qquad \ldots\ldots(1.41)$$

Again making the mapping (1.26), (1.40) is transformed to the polynomial

$$P(z) = \sum_{\nu=0}^{n+1} Q_\nu z^\nu \qquad \ldots\ldots(1.42)$$

with

$$Q_\nu = \binom{n+1}{\nu} - \sum_{\mu=0}^{n} d_\mu \left[\sum_{\xi=0}^{\nu} (-1)^\xi \binom{n-\mu}{\nu-\xi} \binom{\mu+1}{\xi} \right] \quad . \qquad \ldots\ldots(1.43)$$

The sufficient stability condition (1.25) is thus satisfied if (1.42) is a Hurwitz polynomial. The necessary condition (1.24) can usually be proved directly.

The most convenient explicit difference approximations for practical use are, of course, those with $n = 0$, i.e. two-level equations. In all cases with $n \geq 1$ initial computations with some other approximation procedure have to be made in order to determine values $U_{j,k}$ for n initial time-steps before the computation with the actual difference approximation can be started. Due to these practical considerations, only those cases with $n \leq 1$ will be considered.

Par. 1.5 Stability conditions for explicit difference equations with $n \leq 1$, $m \leq 2$.

In this and the remaining paragraphs of this chapter it will be assumed that the difference equations considered are symmetric, i.e. that

$$b_{p,-q} = b_{-p,-q} \;, \quad p = 1,2,\ldots\ldots,m; \; q = 0,1,\ldots\ldots,n. \qquad \ldots\ldots(1.44)$$

Using the results of par. 1.4 it follows that it is necessary and sufficient for the stability of the difference equation (1.35) with $n \leq 1$ that

$$\begin{aligned} Q_0 &= 1 - d_0 - d_1 \\ Q_1 &= 2(1+d_1) \qquad\qquad \ldots\ldots(1.45) \\ Q_2 &= 1 + d_0 - d_1 \end{aligned}$$

given by (1.43) with d_0 and d_1 given by (1.41), have the same sign.

For the case $m \leq 2$ the possible choices for the coefficients $b_{p,-q}$, $b_{0,+1}$ of (1.35) for which the difference equation will be a stable and consistent approximation of (1.1) are given by

Theorem 1.3

If the coefficients $b_{p,-q}$ and $b_{0,+1}$ of (1.35) with $m \leq 2$, $n \leq 1$ are chosen such that

$$b_{0,0} = -(1+2r) + 2b_{0,+1} + 6b_{2,0} + 2b_{1,-1} + 8b_{2,-1} ,$$

$$b_{1,0} = r - 4b_{2,0} - b_{1,-1} - 4b_{2,-1} ,$$

$$b_{0,-1} = 1 - b_{0,+1} - 2b_{1,-1} - 2b_{2,-1} \qquad .....(1.46)$$

and, if

$$b_{0,+1} \neq 1 \quad \frac{\Delta t}{\Delta x} \rightarrow 0 \text{ as } \Delta t \rightarrow 0,$$

and

$$\frac{1}{2} < b_{0,+1} ,$$

$$\frac{1 - 2b_{0,+1}}{4} < b_{1,-1} < \frac{1}{4} ,$$

$$b_{2,-1} < \frac{1 - 2b_{1,-1} + \sqrt{1 - 4b_{1,-1}}}{8}$$

and, if

$$0 < r \leq 2b_{0,+1} - 1 + 2(b_{1,-1} + 4b_{2,-1})$$

then

$$\frac{r - 2b_{1,-1}}{4} - \frac{2b_{0,+1}}{8} - b_{2,-1} \leq b_{2,0} \leq \frac{r}{4} - b_{2,-1} ,$$

whereas, if

$$2b_{0,+1} - 1 + 2(b_{1,-1}+4b_{2,-1}) \leq r \leq$$

$$\leq 2b_{0,+1} - 1+2(b_{1,-1}+4b_{2,-1}) + \sqrt{(2b_{0,+1}-1)(2b_{0,+1}-1+4b_{1,-1})}$$

then

$$\frac{[r - 2(b_{1,-1}+4b_{2,-1})]^2}{8(2b_{0,+1}-1)} + b_{2,-1} \leq b_{2,0} \leq \frac{r}{4} - b_{2,-1} ,$$

$$.....(1.47)$$

then (1.35) will be a consistent and stable approximation of (1.1).

Proof

As the proof is elementary, only an outline is given here.

The conditions (1.46) are derived directly from the consistency conditions (1.36) by putting m = 2, n = 1 and using a Taylor-series expansion.

In order to derive the stability conditions (1.47), (1.45) can be written, using (1.40) and (1.41),

$$Q_0 = \frac{4 \sin^2 \frac{\beta\Delta x}{2}}{b_{0,+1}} [r - 4(b_{2,0}+b_{2,-1}) \sin^2 \frac{\beta\Delta x}{2}] ,$$

$$Q_1 = \frac{2}{b_{0,+1}} [1-4(b_{1,-1}+4b_{2,-1}) \sin^2 \frac{\beta\Delta x}{2} + 16b_{2,-1} \sin^4 \frac{\beta\Delta x}{2}] ,$$

$$Q_2 = \frac{2}{b_{0,+1}} [2b_{0,+1}-1-2\{b_{1,0}-b_{1,-1}+4(b_{2,0}-b_{2,-1})\} \sin^2 \frac{\beta\Delta x}{2} +$$

$$+ 8(b_{2,0}-b_{2,-1}) \sin^4 \frac{\beta\Delta x}{2}] . \qquad .....(1.48)$$

Hence, the polynomial (1.42) is in this case

$$P(z) = Q_2 z^2 + Q_1 z + Q_0$$

and thus, using theorem 1.1 and the results of par. 1.4 it is necessary and sufficient for the stability of the difference equation that the Q_i, i = 0,1,2, have the same sign.

Those cases when the $Q_i = 0$ can be treated in various ways [8] but the easiest method is to use the characteristic equation (1.40) and (1.24), (1.25) directly.

From these conditions the conditions (1.47) are derived through a lengthy but elementary calculation, which will be omitted. This concludes the proof.

A number of results follow from the theorem 1.3. Some of these are well known.

Corollary 1.1

If $n = 0$, $m = 1$, $b_{0,+1} = 1$ in (1.35) the difference equation will be stable only if $0 < r \leq \frac{1}{2}$.

Proof:

If $n = 0$, $m = 1$, $b_{0,+1} = 1$ the consistency conditions (1.46) become

$$\begin{aligned} b_{0,0} &= 1 - 2r, \\ b_{1,0} &= r, \\ b_{0,-1} &= 0. \end{aligned} \qquad \text{.....(1.49)}$$

The first three conditions of (1.47) are automatically satisfied. The restrictions on r give:

i) if $0 < r \leq 1$: $\frac{2r-1}{8} \leq b_{2,0} = 0 \leq \frac{r}{4}$;

ii) if $1 \leq r \leq 2$: $\frac{r^2}{8} \leq b_{2,0} = 0 \leq \frac{r}{4}$,

i.e. the difference equation will be stable only if $0 < r \leq \frac{1}{2}$, see, for example, [3], [17], [20].

Corollary 1.2

If $n = 0$, $m \leq 2$, $b_{0,+1} = 1$ in (1.35) it is only when $0 < r \leq 2$ that it is possible to obtain values for the coefficients of the difference equation for which it will be a consistent and stable approximation of (1.1).

Proof:

With $n = 0$, $m \leq 2$, $b_{0,+1} = 1$ (1.46) becomes

$$\begin{aligned} b_{0,0} &= 1 - 2r + 6b_{2,0}, \\ b_{1,0} &= r - 4b_{2,0} , \\ b_{0,-1} &= 0. \end{aligned} \qquad \text{.....(1.50)}$$

According to (1.47) the approximation will be stable if, for

$$0 < r \leq 1 : \quad \frac{2r-1}{8} \leq b_{2,0} \leq \frac{r}{4}$$

and, for

$$1 \leq r \leq 2 : \quad \frac{r^2}{8} \leq b_{2,0} \leq \frac{r}{4} . \qquad .....(1.51)$$

See also [24] and Fig. 2.

Corollary 1.3

If $n = 1$, $m \leq 2$, $b_{0,+1} = 1$ in (1.35) it is possible to choose the coefficients of the difference equation so that the approximation will be stable for $0 < r < 4$.

Proof:

From (1.47) the maximum value of r for which stability can be obtained, is given by

$$\begin{aligned} r &\leq 1 + 2(b_{1,-1} + 4b_{2,-1}) + \sqrt{1 + 4b_{1,-1}} \\ &< 2 + \sqrt{1 - 4b_{1,-1}} + \sqrt{1 + 4b_{1,-1}} \\ &\leq 4 \end{aligned} \qquad .....(1.52)$$

which maximum is obtained if $b_{1,-1} = 0$.

Corollary 1.4

If $n = 1$, $m \leq 2$ in (1.35) it is possible to choose the coefficients of the difference equation for any value of $r > 0$ so that the equation will be stable.

Proof:

According to (1.47) a stable choice of the coefficients can be made for

$$0 < r \leq 2b_{0,+1} - 1 + 2(b_{1,-1} + 4b_{2,-1}).$$

Thus, if $b_{0,+1}$ is chosen such that the condition

$$\frac{r+1}{2} - (b_{1,-1} + 4b_{2,-1}) \leq b_{0,+1} \qquad .....(1.53)$$

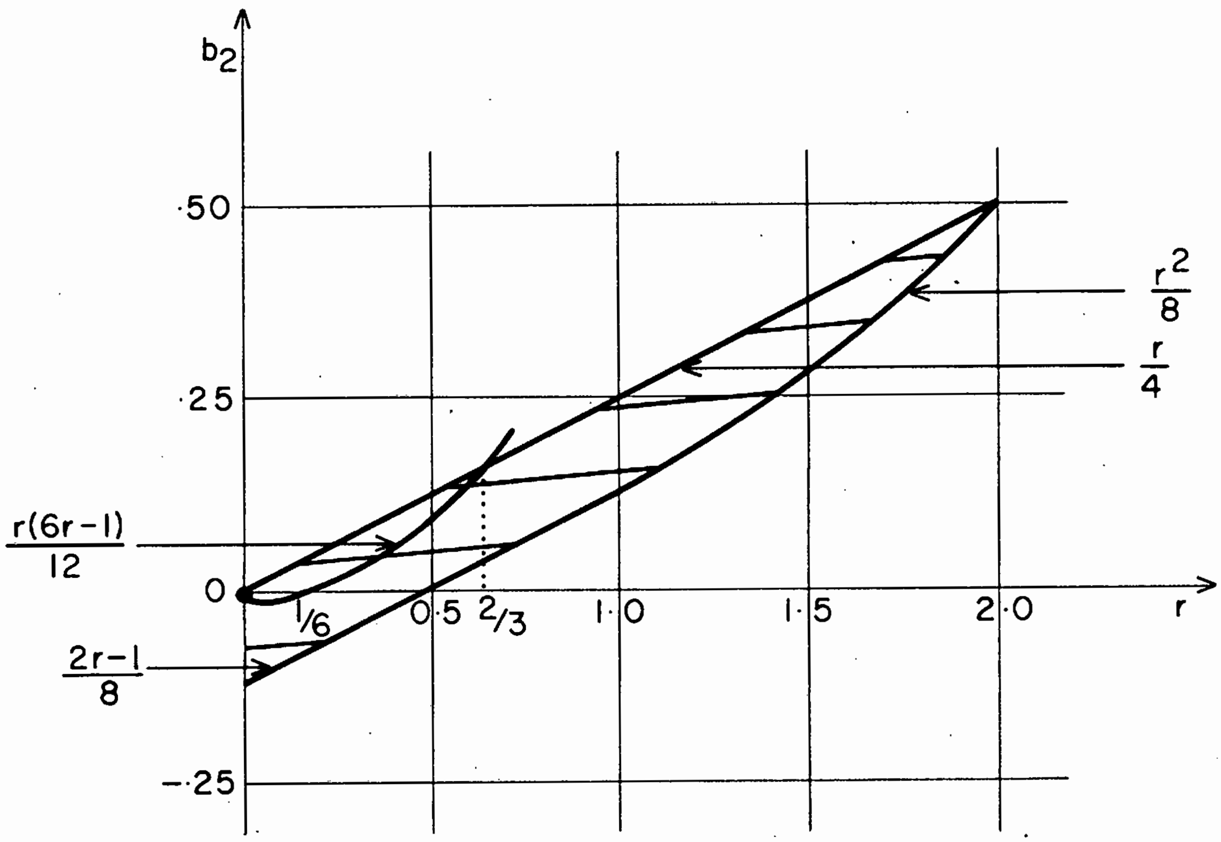

FIGURE 2

XG4-1033

is fulfilled for any permissible values of r, $b_{1,-1}$ and $b_{2,-1}$, the equation will be stable.

The truncation error of (1.35) is determined by the values of the coefficients of the difference equation.

If $n \leq 1$, $m \leq 2$, $b_{0,+1} = 1$ in (1.35), the truncation error is given by

$$E = O(\Delta t) + O((\Delta x)^2) \; . \qquad .....(1.54)$$

Under the assumption that u is sufficiently smooth and using the relations

$$u_{tt} = \sigma^2 u_{xxxx} = \sigma u_{xxt}$$

as before, it follows also by use of a Taylor-series expansion, that if

$$b_{2,0} = \frac{r}{12}(6r+48b_{2,-1}+12b_{1,-1}-1) - b_{2,-1} \qquad .....(1.55)$$

the truncation error reduces to

$$E = O((\Delta t)^2) + O((\Delta x)^4) \; . \qquad .....(1.56)$$

The condition (1.55) has of course to be fulfilled in addition to the conditions of theorem 1.3.

If $b_{0,+1} \neq 1$ an increase in the truncation error results, given by

$$E = O((\frac{\Delta t}{\Delta x})^2) + O((\Delta t)^2) + O((\Delta x)^2) \qquad .....(1.57)$$

and, in order to ensure consistency, the additional assumption has to be made that $\frac{\Delta t}{\Delta x} \to 0$ as Δt, $\Delta x \to 0$.

Par. 1.6 Smoothing formulas for (1.35) with $n = 0$, $m = 2$, $b_{0,+1} = 1$.

With $m = 2$ in (1.35) the difference equation is not defined for all grid points on the time-level $t = (k+1)\Delta t$. This is the same problem as that discussed in par. 1.3, where a special case of (1.35) was considered. Thus the question is whether it is possible at all to construct an algorithm, comprising a suitable basic difference equation and a smoothing formula, which is equivalent to (1.35).

That this is indeed possible will be shown by a number of examples using different basic difference equations. In all cases the smoothing formulas discussed will be of the general form

$$U'_{j,k+1} = \sum_{\ell=-\hat{n}_1}^{\hat{n}_2} \sum_{i=-\hat{m}}^{\hat{m}} a_{i,\ell} \, U_{j+i,k+\ell}, \quad j=1,2,\ldots\ldots,M-1; \quad k=\hat{n}_1,\hat{n}_1+1,\ldots\ldots \tag{1.58}$$

In this the $U_{j,k}$ are computed by use of a suitable basic difference equation, the $a_{i,\ell}$ are suitable constants, $\hat{n}_1$, $\hat{n}_2$ and $\hat{m}$ non-negative integers.

One of the requirements in the construction of suitable smoothing formulas of type (1.58) is of course that they must be defined for all grid points on any time-level, i.e.

$$\hat{m} \leq 1 \ . \tag{1.59}$$

That such an algorithm is not unique, can easily be shown by an example, for instance (1.35) with $n = 0$, $m \leq 2$, $b_{0,+1} = 1$.

As was shown in corollary 1.2 this approximation is stable for $0 < r \leq 2$ if the coefficients of the difference equation comply with the conditions of theorem 1.3 (see Fig. 2). The truncation error is then given by (1.54).

If, in addition, it is required that, from (1.55),

$$b_{2,0} = \frac{r(6r-1)}{12} \ , \tag{1.60}$$

the truncation error is given by (1.56).

<u>Corollary 1.5</u>

If $n = 0$, $m \leq 2$, $b_{0,+1} = 1$ in the difference equation (1.35) and $0 < r \leq \frac{2}{3}$ then it is possible to choose the coefficients of the difference equation in such a way that the condition (1.60) is fulfilled in addition to the conditions of theorem 1.3.

Proof:

It follows trivially that (1.46) and the first three conditions of (1.47) are fulfilled. Furthermore, if $0 < r \leq 1$:

$$\frac{2r-1}{8} \leq b_{2,0} \leq \frac{r}{4}$$

which condition together with (1.60) can be fulfilled for

$$0 < r \leq \frac{2}{3} \quad . \qquad \text{.....(1.61)}$$

In this example two different basic difference equations will be considered, viz. (1.3) and the well-known difference equation (1.34). For this last equation the result of corollary 1.1 holds. For $r > \frac{1}{2}$ the equation (1.34) is thus unstable. In this case the behaviour of the propagated error $\epsilon_{j,k}$ due to initial round-off errors g_j, $j = 1,2,\ldots,M-1$, can be made evident in the following way:

The propagated error must satisfy the following equations (compare case (1.3), par. 1.2):

$$\epsilon_{j,k+1} = r\epsilon_{j-1,k} + (1-2r)\epsilon_{j,k} + r\epsilon_{j+1,k} \qquad \text{.....(1.62)}$$

$$\epsilon_{j,0} = g_j, \qquad \text{.....(1.63)}$$

$$\epsilon_{0,k} = \epsilon_{M,k} = 0. \qquad \text{.....(1.64)}$$

Again, an analytical solution of these equations can be constructed in a way analogous to that used for case (1.3), par. 1.2:

$$\epsilon_{j,k} = \sum_{\nu=1}^{M-1} a_\nu \gamma^k \sin \frac{\nu j \pi}{M} \qquad \text{.....(1.65)}$$

with

$$\gamma = 1 - 4r \sin^2 \frac{\nu\pi}{2M} \quad .$$

As before, the a_ν are constants uniquely determined by the initial conditions (1.63). An explicit formula, involving finite sums of the g_j can be found in [11].

Thus, if

$$r \sin^2 \frac{\nu\pi}{2M} > \frac{1}{2}$$

for one or more of the values of ν between 1 and M-1, then one or more of the terms in (1.65) will grow exponentially with alternating sign with increasing k, unless the corresponding a_ν is zero.

In all solutions of the differential equation computed by use of (1.34) with $r > \frac{1}{2}$ it has been observed that, for increasing k, the error grows exponentially with alternating sign as compared with the analytical solution. (See, for instance, results given by O'Brien, Hyman and Kaplan [17] and Table I).

The following algorithm using (1.34) is now described:

Algorithm 1.2

Step 1: Using (1.34) the values $U_{j,1}$, $j = 1,2,\ldots\ldots,M-1$, are computed from the known values $U_{j,0}$, $j = 0,1,\ldots\ldots,M$, given by (1.4). Using the values $U_{0,1}$ and $U_{M,1}$ given by (1.4) and these computed values $U_{j,1}$, $j = 1,2,\ldots\ldots,M-1$, values $U_{j,2}$, $j = 1,2,\ldots\ldots,M-1$, are then computed. This is repeated for $\hat{n}_2$ cycles (see (1.58)).

Step 2: To these known and computed values on the time-levels $t = 0$, $t = \Delta t$, ..., $t = \hat{n}_2\Delta t$, a smoothing formula of type (1.58) is applied to give values $U'_{j,1}$, $j=1,2,\ldots\ldots,M-1$. It is required that these smoothed values should be good approximations of the solution of the initial boundary value problem (1.1), (1.2).

Step 3: Using these smoothed values for the time-level $t = \Delta t$, step 1 is repeated to give values for $t = 2\Delta t$, $t = 3\Delta t$, ..., $t = (\hat{n}_2+1)\Delta t$. With these values step 2 is repeated to give smoothed values $U'_{j,2}$, $j = 1,2,\ldots\ldots,M-1$. This process can now be repeated for any desired number of cycles.

In this algorithm the following smoothing formula can be used:

Theorem 1.4

Given an approximate solution of the initial boundary value problem (1.1), (1.2) for the time-level $t = k\Delta t$, and values for the time-levels $t = (k+1)\Delta t$, $t = (k+2)\Delta t$ computed according to step 1 of algorithm 1.2, then the smoothing formula (1.58) with $\hat{n}_1 = 0$, $\hat{n}_2 = 2$, $\hat{m} = 1$:

$$U'_{j,k+1} = \sum_{\ell=0}^{2} \sum_{i=-1}^{1} a_{i,\ell} U_{j+i,k+\ell}, \quad j = 1,2,\ldots,M-1, \qquad \ldots(1.66)$$

with the $a_{i,\ell}$ chosen such that the relations

$$a_{-1,\ell} = a_{1,\ell}, \quad \ell = 0,1,2, \qquad \ldots\ldots(1.67)$$

$$a_{1,2} = 0,$$

$$\begin{aligned} b_{0,0} &= a_{0,0} + (1-2r)a_{0,1} + 2ra_{1,1} + [(1-2r)^2+2r^2]a_{0,2} \\ b_{1,0} &= a_{1,0} + r\,a_{0,1} + (1-2r)a_{1,1} + 2r(1-2r)a_{0,2} \\ b_{2,0} &= r\,a_{1,1} + r^2 a_{0,2} \end{aligned} \qquad \ldots\ldots(1.68)$$

with the $b_{p,0}$, $p = 0,1,2$, the coefficients of the difference equation (1.35) with $n = 0$, $m = 2$, $b_{0,+1} = 1$, hold, applied to these values on the time-levels $t = k\Delta t$, $t = (k+1)\Delta t$, $t = (k+2)\Delta t$ according to step 2 of algorithm 1.2, results in a computational procedure which is equivalent to the difference scheme (1.35) with $n = 0$, $m = 2$, $b_{0,+1} = 1$.

Proof:

In accordance with step 1 of algorithm 1.2 the basic difference equation (1.34) is substituted into the right-hand side of the smoothing formula (1.66):

$$U'_{j,k+1} = a_{0,0}\,U_{j,k} + a_{1,0}\,(U_{j-1,k} + U_{j+1,k})$$
$$+ a_{0,1}\,U_{j,k+1} + a_{1,1}\,(U_{j-1,k+1} + U_{j+1,k+1})$$
$$+ a_{0,2}\,U_{j,k+2}\ .$$

This expresses $U'_{j,k+1}$ in terms of values on the time-level $t = k\Delta t$ only:

$$U'_{j,k+1} = [a_{0,0}+(1-2r)a_{0,1}+2ra_{1,1}+(1-4r+6r^2)a_{0,2}]\,U_{j,k}$$
$$+[a_{1,0}+ra_{0,1}+(1-2r)a_{1,1}+2r(1-2r)a_{0,2}](U_{j-1,k}+U_{j+1,k})$$
$$+ r\,[a_{1,1}+ra_{0,2}]\,(U_{j-2,k} + U_{j+2,k})\ .$$

According to the assumptions of the theorem these values are approximate solutions of the differential equation (1.1) considered. Equating the coefficients of this equation with the coefficients of the difference equation (1.35) with $n = 0$, $m = 2$, $b_{0,+1} = 1$:

$$U_{j,k+1} = b_{0,0}\,U_{j,k}+b_{1,0}(U_{j-1,k}+U_{j+1,k}) + b_{2,0}(U_{j-2,k}+U_{j+2,k}) \qquad .....(1.69)$$

give the relations (1.68). The relation (1.67) results from the assumed symmetry (1.44) of the difference equations considered.

From (1.68) it is clear that a number of different possibilities exist for the choice of the smoothing formula. Three of these, chosen at random, are the following:

<u>Formula I</u>

With $a_{0,1} = a_{0,2} = 0$ the smoothing formula is given by

$$U'_{j,k+1} = a_{0,0}\,U_{j,k} + a_{1,0}\,(U_{j-1,k}+ U_{j+1,k})$$
$$+ a_{1,1}\,(U_{j-1,k+1} + U_{j+1,k+1})\ . \qquad .....(1.70)$$

According to (1.68)

$$a_{0,0} = b_{0,0} - 2b_{2,0}$$
$$a_{1,0} = b_{1,0} - \left(\frac{1-2r}{r}\right) b_{2,0} \qquad .....(1.71)$$
$$a_{1,1} = \frac{1}{r}\,b_{2,0}\ .$$

Formula II

With $a_{1,0} = a_{1,1} = 0$ the smoothing formula becomes

$$U'_{j,k+1} = a_{0,0} U_{j,k} + a_{0,1} U_{j,k+1} + a_{0,2} U_{j,k+2} \qquad \ldots\ldots(1.72)$$

with, from (1.68)

$$a_{0,0} = b_{0,0} - (\frac{1-2r}{r}) b_{1,0} + \frac{1}{r^2}(1-4r+2r^2)b_{2,0}$$

$$a_{0,1} = \frac{1}{r} b_{1,0} - \frac{2(1-2r)}{r^2} b_{2,0}$$

$$a_{0,2} = \frac{1}{r^2} b_{2,0} \ . \qquad \ldots\ldots (1.73)$$

Formula III

With $a_{1,0} = a_{0,2} = 0$ the smoothing formula becomes

$$U'_{j,k+1} = a_{0,0} U_{j,k} + a_{0,1} U_{j,k+1} + a_{1,1} (U_{j-1,k+1}+U_{j+1,k+1}) \qquad \ldots\ldots(1.74)$$

with, from (1.68)

$$a_{0,0} = b_{0,0} - (\frac{1-2r}{r}) b_{1,0} + \frac{1}{r^2} (1-4r+2r^2)b_{2,0}$$

$$a_{0,1} = \frac{1}{r} b_{1,0} - (\frac{1-2r}{r^2}) b_{2,0}$$

$$a_{1,1} = \frac{1}{r} b_{2,0} \ . \qquad \ldots\ldots(1.75)$$

To construct a smoothing formula that uses (1.3) as the basic difference equation, the following method can be used, which is very similar to algorithm 1.1:

Algorithm 1.3

Step 1: Using (1.3), the values $U_{j,2}$, $j = 1,2,\ldots\ldots,M-1$, are computed from the known values $U_{0,1}$, $U_{M,1}$ and $U_{j,0}$, $j = 1,2,\ldots\ldots,M-1$, given by (1.4), and the values $U_{j,1}$, $j = 1,2,\ldots\ldots,M-1$, computed by means of another suitable approximation method.

Step 2: To these known and computed values on the time-levels $t = 0$, $t = \Delta t, t = 2\Delta t$ a suitable smoothing formula is applied to give values $U'_{j,2}$, $j = 1,2,\ldots\ldots,M-1$, such that these values are good approximations to the solution of the differential equation.

Step 3: Using the known values on the time-level $t = \Delta t$ and the smoothed values for $t = 2\Delta t$, step 1 is repeated to give values for $t = 3\Delta t$. Then step 2 is repeated to give smoothed values $U'_{j,3}$, $j = 1,2,\ldots\ldots,M-1$. This process can now be repeated for any desired number of cycles.

One possible smoothing formula which can be used in algorithm 1.3 is given by

Theorem 1.5

Given an approximate solution of the initial boundary value problem (1.1), (1.2) for the time-levels $t = (k-1)\Delta t$, $t = k\Delta t$ and values for the time-level $t = (k+1)\Delta t$ computed according to step 1 of algorithm 1.3, then the smoothing formula (1.58) with $\hat{n}_1 = \hat{n}_2 = \hat{m} = 1$, $a_{1,0} = a_{-1,0} = 0$, $a_{-1,-1} = a_{1,-1}$ and $a_{-1,1} = a_{1,1}$:

$$\begin{aligned} U'_{j,k+1} = {} & a_{0,-1} U_{j,k-1} + a_{1,-1} (U_{j-1,k-1} + U_{j+1,k-1}) \\ & + a_{0,0} U_{j,k} + a_{0,1} U_{j,k+1} \\ & + a_{1,1} (U_{j-1,k+1} + U_{j+1,k+1}) \end{aligned} \quad \ldots\ldots(1.76)$$

the a's chosen in such a way that the relations

$$\begin{aligned} b_{0,0} &= a_{0,0} - 4ra_{0,1} + 4ra_{1,1} \\ b_{1,0} &= 2ra_{0,1} - 4ra_{1,1} \\ b_{2,0} &= 2ra_{1,1} \end{aligned} \quad \ldots\ldots(1.77a)$$

and

$$a_{0,-1} + a_{0,1} = a_{1,-1} + a_{1,1} = 0, \quad \ldots\ldots(1.77b)$$

with the $b_{p,0}$, $p = 0,1,2$, the coefficients of the difference equation (1.69), hold, applied to these values on the time-levels $t = (k-1)\Delta t$, $t = k\Delta t$, $t = (k+1)\Delta t$ according to step 2 of algorithm 1.3, results in a computational procedure which is equivalent to the difference schemes (1.69).

Proof:

By substituting (1.3) into the right-hand side of the smoothing formula (1.76) the theorem can be proved in the same way as theorem 1.4.

The smoothing formulas given by theorems 1.4 and 1.5 are defined for three consecutive grid points along the x-axis. Thus the algorithms 1.2 and 1.3 are defined for all grid points on the time-level $t = (k+1)\Delta t$ if these smoothing formulas are used respectively. However, as was mentioned in par. 1.3 in connection with theorem 1.2, if these methods are used to compute values near the boundaries, the conditions of the theorems might be violated in that the boundary values are given by (1.4) instead of being computed by (1.3) for instance in the case of $U_{0,k+1}$ and $U_{M,k+1}$.

An analysis similar to that made in the case of theorem 1.2 (p. 22) can be made here. The results thus obtained, viz. that the use of better approximations to the solution of the differential equation than the values given by the basic difference equation used, should not impair the accuracy of the results obtained by use of the method of theorem 1.4, are substantiated by computed results (see, for example, Table II).

In the case of the method of theorem 1.5 results similar to those for theorem 1.4 can be deduced.

According to theorems 1.4 and 1.5 the difference approximation (1.69) can be written as a combination of a number of different smoothing formulas with different basic difference equations.

In order to get an idea of the amount of work involved in computing an approximate solution by one of these methods, a comparison can be made with the ordinary explicit difference equation (1.34). To this end it is convenient to keep Δx (and thus M) constant. Hence, in order to cater for different values of r, Δt is varied. For the sake of such a comparison, a smoothing formula is used to compute values for only those grid points on the time-level $t = (k+1)\Delta t$ for which the difference equation (1.69) is not defined, as was suggested for the method of par. 1.3.

Using the same r (or time-step) in all the cases, it is easily seen that the procedures using the smoothing formulas I, II and III and that of theorem 1.5 require about half as much work again as (1.34). On the other hand, if the maximum possible time-step is used in each case, these smoothing procedures require only about 40% as much work as (1.34).

According to corollary 1.5 it is possible for all $0 < r \leq \frac{2}{3}$ to choose the coefficients of the difference equation (1.69) in such a way that the truncation error is

$$E = O((\Delta t)^2) + O((\Delta x)^4) .$$

As was mentioned before, the same truncation error is obtained for (1.34) if $r = \frac{1}{6}$. Estimates of the relative amounts of work required will be the same as above.

If ease of use is taken into account, the methods of theorem 1.4 are to be preferred. Of the methods given in formulas I, II and III that of formula I is the simplest.

Examples of numerical results obtained by the above-mentioned methods are given in Table II. The problem is the same as that considered in Table I - see par. 1.3.

In all examples Δx was again kept fixed at 0.1 and Δt changed to cater for different values of r. Again all the results

TABLE II

t	Analytical solution	Approx. solution using (1.34),(1.70) r = 0.5 $b_{2,0}$ = 0.083 333 $E=0((\Delta t)^2)+0((\Delta x)^4)$	Approx. solution using (1.34),(1.70) r = 0.6 $b_{2,0}$ = 0.13 $E=0((\Delta t)^2)+0((\Delta x)^4)$	Approx. solution using (1.34),(1.70) r = 1.0 $b_{2,0}$ = 0.2 $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (1.34),(1.72) r = 1.0 $b_{2,0}$ = 0.2 $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (1.34),(1.74) r = 1.0 $b_{2,0}$ = 0.2 $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (1.3),(1.76) r = 1.0 $b_{2,0}$ = 0.2 $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (1.34),(1.70) r = 1.5 $b_{2,0}$ = 0.337 5 $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (1.34),(1.70) r = 2.0 $b_{2,0}$ = 0.5 $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (1.34),(1.70) r = 2.5 $b_{2,0}$ = 0.5 $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (1.34),(1.70) r = 1.0 $b_{2,0}$ = 0.3 $E=0(\Delta t)+0((\Delta x)^2)$
0.00	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000
0.01	.919 331	.920 000		.920 000	.920 000	.920 000	.920 012				.920 000
0.02	.840 708	.840 687		.840 000	.840 000	.840 000	.840 333		.840 000		.840 000
0.03	.764 897	.764 834	.764 832	.761 280	.761 280	.761 280	.762 800	.760 000			.764 320
0.04	.694 326	.694 291		.688 960	.688 960	.688 960	.688 645		.680 000		.695 119
0.05	.629 614	.629 602		.623 040	.623 040	.623 040	.622 059			.600 000	.633 359
0.06	.570 664	.570 668	.570 697	.563 315	.563 315	.563 315	.560 694	.556 521	.540 000		.579 738
0.07	.517 124	.517 137		.509 273	.509 273	.509 273	.506 141				.535 327
0.08	.468 561	.468 580		.460 405	.460 405	.460 405	.456 149		.450 000		.502 120
0.09	.424 540	.424 563	.424 601	.416 221	.416 221	.416 221	.411 713	.407 747			.483 757
0.10	.384 647	.384 673		.376 277	.376 277	.376 277	.371 062		.350 000	.429 999	.486 635
0.11	.348 500	.348 527		.340 166	.340 166	.340 166	.334 892				.521 729
0.12	.315 749	.315 777	.315 815	.307 520	.307 520	.307 520	.301 842	.298 868	.297 500		.607 617
0.13	.286 074	.286 103		.278 007	.278 007	.278 007	.272 404				.775 518
0.14	.259 189	.259 218		.251 327	.251 327	.251 327	.245 534		.226 250		1.077 682
0.15	.234 830	.234 859	.234 894	.227 207	.227 207	.227 207	.221 576	.219 119		.587 497	1.601 374
0.16	.212 760	.212 788		.205 401	.205 401	.205 401	.199 729		.197 500		2.492 166
0.17	.192 764	.192 792		.185 689	.185 689	.185 689	.180 233				3.992 737
0.18	.174 648	.174 675	.174 707	.167 868	.167 868	.167 868	.162 469	.160 674	.145 313		6.507 516
0.19	.158 234	.158 261		.151 758	.151 758	.151 758	.146 604				
0.20	.143 363	.143 389		.137 194	.137 194	.137 194	.132 160		.132 031	1.731 863	

give the computed change in temperature for increasing t at $x = 0.5$.

As in Table I the analytical solution is given in the second column. For $r = 1.0$ the results given have been computed by the methods of formulas I, II, III and theorem 1.5. For all other values of r only results computed by formula I are given.

On comparing these results with those computed with (1.34) for $r = \frac{1}{6}$ and $r = 0.5$ and given in Table I, it will be seen that the results computed for $r = 0.5$ and $r = 0.6$ (third and fourth columns of Table II) compare favourably with those. To compute a solution by the method of formula I for $r = 0.6$, requires less than 50% of the amount of work needed to compute the same solution with (1.34) with $r = \frac{1}{6}$.

Par. 1.7 A smoothing formula for (1.35) with $n = 1$, $m = 2$

In Table III are given a number of explicit difference approximations of type (1.35) with $n = 1$, $m = 2$, $b_{0,+1} = 1$ which can be used to approximate the differential equation (1.1). In each case the respective range of r for which stability can be obtained, is given.

In all these cases as well as in those cases with $n = 1$, $m = 2$, $b_{0,+1} \neq 1$ (see corollary 1.4) the following smoothing procedure can be used:

As the basic difference equation consider (1.35) with $n = 1$, $m = 1$, $b_{0,+1} = 1$, $b_{1,0} = 0$. The range of r for which this equation will be stable is given by

Corollary 1.6

If $n = 1$, $m = 1$, $b_{0,+1} = 1$, $b_{1,0} = 0$ in (1.35) the difference equation will be a consistent approximation of (1.1) which will be stable for $0 < r < \frac{1}{4}$.

Proof:

According to the consistency conditions (1.46) of theorem 1.3 the difference equation (1.35) with n = 1, m = 1, $b_{0,+1} = 1$, $b_{1,0} = 0$ will be a consistent approximation of (1.1) if

$$b_{0,0} = 1,$$

$$b_{0,-1} = -2r,$$

$$b_{1,-1} = r.$$

The stability conditions (1.47) can be satisfied for all $0 < r < \frac{1}{4}$.

Thus the basic difference equation is

$$U_{j,k+1} = U_{j,k} - 2rU_{j,k-1} + r(U_{j-1,k-1} + U_{j+1,k-1}). \qquad \ldots\ldots(1.78)$$

In this case algorithm 1.1 can be used, the only difference being that (1.78) is used instead of the difference equation (1.3). A smoothing formula that can be used in the second step of this algorithm is:

Theorem 1.6

Given an approximate solution of the differential equation (1.1), (1.2) for the time-levels $t = (k-1)\Delta t$, $t = k\Delta t$ and values for the time-levels $t = (k+1)\Delta t$, $t = (k+2)\Delta t$ computed according to step 1 of algorithm 1.1 with (1.78), then the smoothing formula (1.58) with $\hat{n}_1 = 1$, $\hat{n}_2 = 2$, $\hat{m} = 1$:

$$U'_{j,k+1} = \sum_{\ell=-1}^{2} \sum_{i=-1}^{1} a_{i,\ell}\, U_{j+i,k+\ell}$$

and with

$$
\begin{aligned}
a_{0,2} &= 0 \\
a_{-1,2} = a_{1,2} &= \frac{1}{r}\,\hat{b}_{2,0} \\
a_{0,1} &= 0 \\
a_{-1,1} = a_{1,1} &= -\frac{1}{r}\,(\hat{b}_{2,0} - \hat{b}_{2,-1}) \\
a_{0,0} &= \hat{b}_{0,0} - 2\hat{b}_{2,0} \\
a_{-1,0} = a_{1,0} &= \hat{b}_{1,0} + 2\hat{b}_{2,0} - \frac{1}{r}\,\hat{b}_{2,-1} \\
a_{0,-1} &= \hat{b}_{0,-1} - 2\hat{b}_{2,-1} \\
a_{-1,-1} = a_{1,-1} &= \hat{b}_{1,-1} + 2\hat{b}_{2,-1} ,
\end{aligned}
\qquad \text{.....(1.79)}
$$

the $\hat{b}_{p,-q} = \dfrac{b_{p,-q}}{b_{0,+1}}$ being the coefficients of the difference equation (1.35) with $n = 1$, $m = 2$ applied to these values on the time-levels $t = (k-1)\Delta t$, $t = k\Delta t$, $t = (k+1)\Delta t$, $t = (k+2)\Delta t$ according to step 2 of algorithm 1.1, results in a computational procedure which is equivalent to the difference scheme (1.35) with $n = 1$, $m = 2$.

Proof:

This theorem can be proved in the same way as theorem 1.4 by substituting (1.78) into the right-hand side of the smoothing formula, and equating the coefficients with those of the difference equation (1.35).

For use in practical problems, the same remarks apply as were made in connection with the methods given in par. 1.3 and par. 1.6.

With $n = 1$, $m = 2$ the choice (1.55) for $b_{2,0}$ can be made, which condition has to hold subject to the stability conditions (1.47) of theorem 1.3. This leads to the result

Corollary 1.6

If $n = 1$, $m = 2$, $b_{0,+1} = 1$ in the difference equation (1.35) it is possible for all $0 < r < \frac{5+3\sqrt{2}}{6}$ ($\approx 1.540\ 440$) to choose the coefficients of the difference equation so that the condition (1.55) is fulfilled in addition to the conditions of theorem 1.3. In this case the truncation error is given by

$$E = O((\Delta t)^2) + O((\Delta x)^4).$$

Proof:

This result can be deduced directly by comparing (1.55) with the stability conditions (1.47) of theorem 1.3.

An elementary calculation leads to the result, for the case when

$$0 < r \leq 1 + 2(b_{1,-1} + 4b_{2,-1})$$

in theorem 1.3, that, if

a) $0 < r \leq \frac{5}{6}$, then

i) $-\frac{1}{4} < b_{1,-1} < \frac{1}{4}$

ii) $\text{Max}\left[\frac{r-1-2b_{1,-1}}{8}, \frac{-12r^2+8r-3-12(1+2r)b_{1,-1}}{96r}\right] \leq$

$$\leq b_{2,-1} \leq \frac{2-3r-6b_{1,-1}}{24},$$

iii) $$b_{2,0} = \frac{6r^2+(48b_{2,-1} + 12b_{1,-1}-1)r}{12} - b_{2,-1} \quad . \qquad \text{.....(1.80)}$$

For the case

$$1 + 2(b_{1,-1}+4b_{2,-1}) \leq r \leq 1 + 2(b_{1,-1}+4b_{2,-1}) + \sqrt{1+4b_{1,-1}}$$

the result is obtained that, if

b) $\frac{5}{6} < r$, then

i) $\frac{9r^2 - 15r + 4}{9} \le b_{1,-1} < \frac{1}{4}$

ii) $\frac{-3(1-3r+2b_{1,-1}) - \sqrt{3(36r^2-20r+3+12b_{1,-1})}}{24} \le$

$\le b_{2,-1} \le \frac{2-3r-6b_{1,-1}}{24}$

iii) $b_{2,0} = \frac{6r^2+(48b_{2,-1}+12b_{1,-1}-1)r}{12} - b_{2,-1}$.

.....(1.81)

The condition (i) in (1.81) can be satisfied for all

$$r < \frac{5+3\sqrt{2}}{6} \ (\approx 1.540\ 440) \qquad .....(1.82)$$

which concludes the proof.

A comparison, similar to that of par. 1.6, can be made here of the work required to carry out a computation by the method of theorem 1.6. Considering only the methods a , b and e of Table III, and assuming the same time-step is used in every case, about 3 times, 2.5 times and twice as much work is required by these methods as compared with that for the standard explicit method (1.34). If, however, the maximum possible time-step is used in every instance, these factors are roughly $\frac{3}{8}$, $\frac{5}{16}$ and $\frac{1}{4}$ respectively.

According to (1.81) (i) $b_{1,-1}$ can be made zero for all $r \le \frac{4}{3}$. From the consistency conditions (1.46) of theorem 1.3, $b_{1,0}$ can simultaneously be chosen to be zero on condition that $b_{2,0}$ is chosen such that

$$b_{2,0} = \frac{r - 4b_{2,-1}}{4} ,$$

i.e.

$$b_{2,-1} = \frac{2 - 3r}{24} .$$

Thus for $0 < r \leq \frac{4}{3}$ it is possible to choose $b_{1,-1} = b_{1,0} = 0$ and still retain the smaller truncation error given in corollary 1.6, which is of the same order as the truncation error of (1.34) with $r = \frac{1}{6}$. The computation for this approximation ((1.34) with $r = \frac{1}{6}$) requires 4 times as much work as that for Table III, e with $r = \frac{4}{3}$.

In Table IV are given results computed by methods a and e from Table III. The problem is the same as that considered in Tables I and II. The remarks made previously on the choice of the difference grid,apply in this case also.

The methods used to compute these results were chosen with the view of using a good approximation which does not involve an excessive amount of work. A disadvantage of all these methods is that initial values on two consecutive time-levels are required. In the results given, (1.34) with $r = \frac{1}{6}$ was used to compute the second line of initial values.

In the case of the method given in Table III, e it is of course not necessary to use a smoothing formula in order to compute a solution, but then a solution is not obtained for all grid points.

Par. 1.8 <u>The difference equation (1.35) with $b_{0,+1} \neq 1$</u>

As was mentioned in corollary 1.4 of par. 1.5 it is possible so to choose the coefficients of the difference equation (1.35) that the approximation will be stable for all possible choices of the difference grid. Two examples of equations of this type will be given here.

As a first example consider (1.35) with $n = m = 1$, $b_{0,0} = b_{1,-1} = 0$. This implies that the following conditions have to be fulfilled by the coefficients of the difference equation:

TABLE IV

t	Analytical solution	Approx. solution using Table IIIe $r = 0.5$ $b_{0,0} = 0.791\ 667$ $b_{1,0} = 0.0$ $b_{2,0} = 0.104\ 167$ $b_{0,-1} = -0.041\ 667$ $b_{1,-1} = 0.0$ $b_{2,-1} = 0.020\ 833$ $E = O((\Delta t)^2) + O((\Delta x)^4)$	Approx. solution using Table IIIe $r = 1.0$ $b_{0,0} = 0.416\ 667$ $b_{1,0} = 0.0$ $b_{2,0} = 0.291\ 667$ $b_{0,-1} = 0.083\ 333$ $b_{1,-1} = 0.0$ $b_{2,-1} = -0.041\ 667$ $E = O((\Delta t)^2) + O((\Delta x)^4)$	Approx. solution using Table IIIa $r = 1.5$ $b_{0,0} = 0.364\ 444$ $b_{1,0} = -0.215\ 556$ $b_{2,0} = 0.533\ 333$ $b_{0,-1} = -0.124\ 444$ $b_{1,-1} = 0.222\ 222$ $b_{2,-1} = -0.16$ $E = O((\Delta t)^2) + O((\Delta x)^4)$	Approx. solution using Table IIIe $r = 2.0$ $b_{0,0} = 0.020\ 833$ $b_{1,0} = 0.0$ $b_{2,0} = 0.489\ 583$ $b_{0,-1} = -0.020\ 833$ $b_{1,-1} = 0.0$ $b_{2,-1} = 0.010\ 417$ $E = O(\Delta t) + O((\Delta x)^2)$	Approx. solution using Table IIIe $r = 3.0$ $b_{0,0} = -0.25$ $b_{1,0} = 0.0$ $b_{2,0} = 0.625$ $b_{0,-1} = -0.25$ $b_{1,-1} = 0.0$ $b_{2,-1} = 0.125$ $E = O(\Delta t) + O((\Delta x)^2)$	Approx. solution using Table IIIe $r = 3.75$ $b_{0,0} = -0.437\ 5$ $b_{1,0} = 0.0$ $b_{2,0} = 0.718\ 75$ $b_{0,-1} = -0.437\ 5$ $b_{1,-1} = 0.0$ $b_{2,-1} = 0.218\ 75$ $E = O(\Delta t) + O((\Delta x)^2)$
0.00	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000
0.01	.919 331	.920 004	.920 003				
0.02	.840 708	.840 775	.840 353		.840 885		
0.03	.764 897	.764 938	.764 047	.762 947		.764 705	
0.04	.694 326	.694 383	.694 191		.687 479		
0.05	.629 614	.629 678	.629 574				
0.06	.570 664	.570 730	.570 935	.570 460	.553 175	.545 764	
0.07	.517 124	.517 188	.517 468				
0.08	.468 561	.468 622	.469 010		.446 973		
0.09	.424 540	.424 598	.425 020	.425 773		.367 845	
0.10	.384 647	.384 702	.385 158		.361 704		
0.11	.348 500	.348 551	.349 018				
0.12	.315 749	.315 796	.316 271	.317 734	.291 732	.250 131	
0.13	.286 074	.286 118	.286 592				
0.14	.259 189	.259 229	.259 698		.236 252		
0.15	.234 830	.234 868	.235 327	.237 154		.187 540	.133 495
0.16	.212 760	.212 795	.213 244		.190 442		
0.17	.192 764	.192 797	.193 232				
0.18	.174 648	.174 678	.175 099	.176 879	.154 316	.113 432	
0.19	.158 234	.158 262	.158 667				
0.20	.143 363	.143 389	.143 777		.124 310		

From the consistency conditions (1.46):

i) $b_{0,0} = -(1+2r) + 2b_{0,+1}$

ii) $b_{1,0} = r$ .....(1.83)

iii) $b_{0,-1} = 1 - b_{0,+1}$

and from the stability conditions (1.47):

iv) $\frac{1}{2} < b_{0,+1}$

v) a) <u>if $0 < r \leq 2b_{0,+1} - 1$:</u>

$r + \frac{1}{2} \leq b_{0,+1}$

b) <u>if $2b_{0,+1} - 1 \leq r \leq 2(2b_{0,+1} - 1)$:</u>

$$\frac{1}{2b_{0,+1} - 1} \leq 0 \text{ .} \qquad .....(1.84)$$

The condition v) b) can clearly not be satisfied. If $b_{0,+1}$ is chosen so that

$$b_{0,+1} \geq r + \frac{1}{2} \qquad .....(1.85)$$

the stability conditions (1.84) will be satisfied for all $r > 0$. The remaining coefficients of the difference equation are then given by (1.83).

If $b_{0,+1} = r + \frac{1}{2}$ is chosen, the difference equation is simply the well-known Du Fort-Frankel equation [5], [7], [20]:

$$\frac{U_{j,k+1} - U_{j,k-1}}{2\Delta t} = \sigma \frac{U_{j-1,k} - U_{j,k+1} - U_{j,k-1} + U_{j+1,k}}{(\Delta x)^2} \text{ .} \qquad .....(1.86)$$

A second example is given by (1.35) with $n = 1$, $m = 2$, $b_{1,-1} = b_{2,-1} = 0$. This choice results in the following relations for the coefficients of the difference equation:
From (1.46):

i) $b_{0,0} = -(1+2r) + 2b_{0,+1} + 6b_{2,0}$

ii) $b_{1,0} = r - 4b_{2,0}$ .....(1.87)

iii) $b_{0,-1} = 1 - b_{0,+1}$

and from (1.47):

iv) $\frac{1}{2} < b_{0,+1}$

v) a) <u>if $0 < r \leq 2b_{0,+1} - 1$:</u>

$$\frac{r}{4} - \frac{2b_{0,+1}-1}{8} \leq b_{2,0} \leq \frac{r}{4}$$

b) <u>if $2b_{0,+1}-1 \leq r \leq 2(2b_{0,+1}-1)$:</u>

$$\frac{r^2}{8(2b_{0,+1}-1)} \leq b_{2,0} \leq \frac{r}{4} \quad . \qquad \text{.....(1.88)}$$

In this case also it is possible to choose the coefficients so that the difference approximation will be stable for any values of r.

For both examples the truncation error is given by (1.57):

$$E = O((\frac{\Delta t}{\Delta x})^2) + O((\Delta t)^2) + O((\Delta x)^2).$$

Thus, in order to ensure consistency, it has to be required that $\frac{\Delta t}{\Delta x} \rightarrow 0$ as $\Delta t, \Delta x \rightarrow 0$ (see theorem 1.3).

Results computed with these two examples are given in Table V. The problem which was previously considered, is considered here also.

If compared with the results given in Tables I, II and IV it will be noticed that the approximation error increases markedly as r increases, the Du Fort-Frankel approximation giving the worst results.

The smoothing formula of theorem 1.6 can be used directly in the case of the second example, as was done in the computation of the results of Table V.

TABLE V

t	Analytical solution	Approx. solution using Du Fort-Frankel difference approximation. $r = 0.5$ $E = 0(\Delta t) + 0((\Delta x)^2)$	Approx. solution using (1.35) with $m = 2$, $n = 1$. $r = 0.5$ $b_{0,0} = b_{1,0} = 0.0$ $b_{2,0} = 0.125$ $b_{0,-1} = 0.375$ $b_{1,-1} = b_{2,-1} = 0.0$ $b_{0,+1} = 0.625$ $E = 0((\frac{\Delta t}{\Delta x})^2) + 0((\Delta t)^2) + 0((\Delta x)^2)$	Approx. solution using Du Fort-Frankel difference approximation. $r = 1.0$ $E = 0((\frac{\Delta t}{\Delta x})^2) + 0((\Delta t)^2) + 0((\Delta x)^2)$	Approx. solution using (1.35) with $m = 2$, $n = 1$. $r = 1.0$ $b_{0,0} = b_{1,0} = 0.0$ $b_{2,0} = 0.25$ $b_{0,-1} = 0.25$ $b_{1,-1} = b_{2,-1} = 0.0$ $b_{0,+1} = 0.75$ $E = 0((\frac{\Delta t}{\Delta x})^2) + 0((\Delta t)^2) + 0((\Delta x)^2)$	Approx. solution using Du Fort-Frankel difference approximation. $r = 1.5$ $E = 0((\frac{\Delta t}{\Delta x})^2) + 0((\Delta t)^2) + 0((\Delta x)^2)$	Approx. solution using (1.35) with $m = 2$, $n = 1$. $r = 1.5$ $b_{0,0} = b_{1,0} = 0.0$ $b_{2,0} = 0.375$ $b_{0,-1} = 0.125$ $b_{1,-1} = b_{2,-1} = 0.0$ $b_{0,+1} = 0.875$ $E = 0((\frac{\Delta t}{\Delta x})^2) + 0((\Delta t)^2) + 0((\Delta x)^2$	Approx. solution using Du Fort-Frankel difference approximation. $r = 2.0$ $E = 0((\frac{\Delta t}{\Delta x})^2) + 0((\Delta t)^2) + 0((\Delta x)^2)$	Approx. solution using (1.35) with $m = 2$, $n = 1$. $r = 2.0$ $b_{0,0} = b_{1,0} = 0.0$ $b_{2,0} = 0.5$ $b_{0,-1} = 0.0$ $b_{1,-1} = b_{2,-1} = 0.0$ $b_{0,+1} = 1.0$ $E = 0(\Delta t) + 0((\Delta x)^2)$	Approx. solution using Du Fort-Frankel difference approximation. $r = 3.0$ $E = 0((\frac{\Delta t}{\Delta x})^2) + 0((\Delta t)^2) + 0((\Delta x)^2)$	Approx. solution using (1.35) with $m = 2$, $n = 1$. $r = 3.0$ $b_{0,0} = b_{1,0} = 0.0$ $b_{2,0} = 0.75$ $b_{0,-1} = -0.25$ $b_{1,-1} = b_{2,-1} = 0.0$ $b_{0,+1} = 1.25$ $E = 0((\frac{\Delta t}{\Delta x})^2) + 0((\Delta t)^2) + 0((\Delta x)^2)$
0.00	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000
0.01	.919 331	.920 000	.920 008	.920 012	.920 012						
0.02	.840 708	.840 137	.842 469	.840 108	.840 497			.840 885	.840 885		
0.03	.764 897	.762 671	.769 116	.760 670	.765 060	.760 701	.762 399			.764 705	.764 705
0.04	.694 326	.690 796	.700 827	.682 936	.696 591			.683 332	.687 620		
0.05	.629 614	.625 160	.637 877	.609 505	.630 990						
0.06	.570 664	.565 577	.580 194	.543 673	.574 550	.531 028	.565 584	.530 355	.554 131	.534 085	.545 862
0.07	.517 124	.511 608	.527 525	.487 577	.519 119						
0.08	.468 561	.462 767	.479 533	.436 732	.473 185			.387 486	.448 870		
0.09	.424 540	.418 582	.435 856	.391 913	.426 763	.345 900	.418 341			.315 221	.368 278
0.10	.384 647	.378 612	.396 136	.351 025	.389 547			.263 062	.363 068		
0.11	.348 500	.342 459	.360 028	.314 872	.350 742						
0.12	.315 749	.309 757	.327 213	.281 900	.320 678	.233 096	.309 378	.166 819	.293 651	.118 269	.248 008
0.13	.286 074	.280 178	.297 395	.252 789	.288 214						
0.14	.259 189	.253 423	.270 302	.226 296	.264 011			.107 211	.237 693		
0.15	.234 830	.229 224	.245 687	.202 964	.236 790	.154 899	.228 841			-.043 277	.172 454
0.16	.212 760	.207 335	.223 324	.181 717	.217 394			.063 959	.192 159		
0.17	.192 764	.187 536	.203 008	.162 982	.194 499						
0.18	.174 648	.169 628	.184 551	.145 918	.179 050	.100 892	.169 324	.032 784	.155 603	-.154 057	.112 330
0.19	.158 234	.153 430	.167 783	.130 871	.159 718						
0.20	.143 363	.138 779	.152 551	.117 168	.147 512			.009 274	.125 741		

CHAPTER II

A DIFFERENCE APPROXIMATION METHOD, WHICH IS STABLE FOR ANY GRID USED, OF THE ONE-DIMENSIONAL DIFFUSION EQUATION

Par. 2.1 INTRODUCTION

In the methods described in chapter I two cycles at most were computed with a basic difference equation before the application of a smoothing formula. The reason for this is that in the difference equation (1.35) m had to be ≤ 2, as the method used there to determine stability conditions cannot in general be applied to cases with larger values of m. This is due to the fact that conditions have to be derived according to which the coefficients of a polynomial of degree higher than the second can be chosen in such a way that the polynomial will be positive (or negative) over a given interval of the independent variable. There are a number of methods that can (theoretically) be used to derive such conditions [6], [16]. In practical applications it was, however, found that all these methods give stability conditions which are much stronger than necessary.

In view of the advantages of the smoothing technique according to the results of chapter I, the question arises as to whether it is possible to extend this technique in such a way that $m > 2$ cycles are computed with a basic difference equation before application of a smoothing formula. Even weaker stability conditions might be obtained. This implies, however, that the stability of difference equations with $m > 2$ must be established. In order to do this a result given by Forsythe and Wasow ([7], pp. 107 - 113) can be used. This result holds for their definition of stability, definition 0.1, and the maximum norm rather than the Hilbert norm used by Lax and Richtmyer in their analysis [14], [20]. For a of (2.1)

$$b_\nu = 0, \qquad \nu = \pm 2, \pm 3, \ldots, \pm(m-1). \qquad \ldots\ldots(2.3)$$

This reduces (2.1) to the simple equation

$$U_{j,k+1} = b_0 U_{j,k} + b_1 (U_{j-1,k} + U_{j+1,k}) + b_m (U_{j-m,k} + U_{j+m,k}). \qquad \ldots\ldots(2.4)$$

As before, Taylor-series can be used in an elementary calculation to deduce consistency conditions in this case. This leads to the result that, in order to ensure consistency, the relations

$$b_0 + 2b_1 + 2b_m = 1 \qquad \ldots\ldots(2.5)$$

$$b_1 + m^2 b_m = r$$

must hold as $\Delta t \to 0$. With (2.5) satisfied, the truncation error is

$$E = 0(\Delta t) + 0((\Delta x)^2). \qquad \ldots\ldots(2.6)$$

Now assume that b_0 and b_1 are used to satisfy these conditions i.e.

$$b_0 = 1 - 2r + 2(m^2-1)\, b_m \qquad \ldots\ldots(2.7)$$

$$b_1 = r - m^2 b_m .$$

According to theorem 2.1 the difference equation (2.4) will be stable if it is of positive type, which will be the case if, from (2.7)

$$1 - 2r + 2(m^2-1)\, b_m \geq 0,$$

$$r - m^2\, b_m \geq 0,$$

$$b_m \geq 0.$$

These conditions will be satisfied if, with $m > 1$,

$$\text{Max}\left[0, \frac{2r-1}{2(m^2-1)}\right] \leq b_m \leq \frac{r}{m^2} . \qquad \ldots\ldots(2.8)$$

The equation (2.4) will thus be a consistent and stable approximation of the differential equation (1.1) if the relations (2.7) and (2.8) hold.

Theorem 2.2

The coefficients of the difference equation (2.4) can be chosen in such a way that the equation will be a consistent and stable approximation of the differential equation (1.1) for all r such that $0 < r \le \frac{m^2}{2}$.

Proof:

From (2.7)

$$\frac{2r-1}{2(m^2-1)} \le \frac{r}{m^2}$$

or

$$0 < r \le \frac{m^2}{2}. \qquad \text{.....(2.9)}$$

As in chapter I, it may be assumed that the solution of the differential equation (1.1) is sufficiently smooth for the higher order derivatives u_{tt} and u_{xxxx} to exist. Then the fact that u also solves the equation $u_{tt} = \sigma^2 u_{xxxx}$ can be used together with a Taylor-series expansion to yield the result that the truncation error is given by

$$E = 0((\Delta t)^2) + 0((\Delta x)^4) \qquad \text{.....(2.10)}$$

if

$$b_m = \frac{r(6r-1)}{m^2(m^2-1)}. \qquad \text{.....(2.11)}$$

This condition must hold in addition to the consistency and stability conditions (2.7) and (2.8).

This leads to the following result:

Theorem 2.3

If r is chosen such that, if $1 < m \le 3$, then

$$\frac{1}{6} \le r \le \frac{m^2}{6}$$

whereas, if $3 < m$, then either

$$\frac{1}{6} \le r \le \frac{1+m^2-\sqrt{1-10m^2+m^4}}{12}$$

or

$$\frac{1 + m^2 + \sqrt{1-10m^2+m^4}}{12} \le r \le \frac{m^2}{6} , \qquad \ldots\ldots(2.12)$$

then the coefficient b_m of the difference equation (2.1) can be so chosen that (2.11) holds.

Proof:

According to (2.8) and (2.11) three inequalities must be satisfied:

a) $0 \le \frac{r(6r-1)}{m^2(m^2-1)}$ or $\frac{1}{6} \le r$

b) $\frac{r(6r-1)}{m^2(m^2-1)} \le \frac{r}{m^2}$ or $r \le \frac{m^2}{6}$

c) $\frac{2r-1}{2(m^2-1)} \le \frac{r(6r-1)}{m^2(m^2-1)}$.

For $m \le 3$ this inequality holds. If $m \ge 4$ the inequality holds if either

$$r \le \frac{1 + m^2 - \sqrt{1-10m^2+m^4}}{12}$$

or

$$\frac{1 + m^2 + \sqrt{1-10m^2+m^4}}{12} \le r .$$

(See Fig. 3).

As a final remark, consider the following two examples of the difference equation (2.1):

a) Let $m=2$, $b_m = 0$ in (2.1):

The consistency conditions (2.7) then give

$$b_0 = 1 - 2r,$$

$$b_1 = r,$$

thus the equation will be of positive type if

$$r \le \frac{1}{2} .$$

Thus (2.1) simply becomes the explicit equation (1.34).

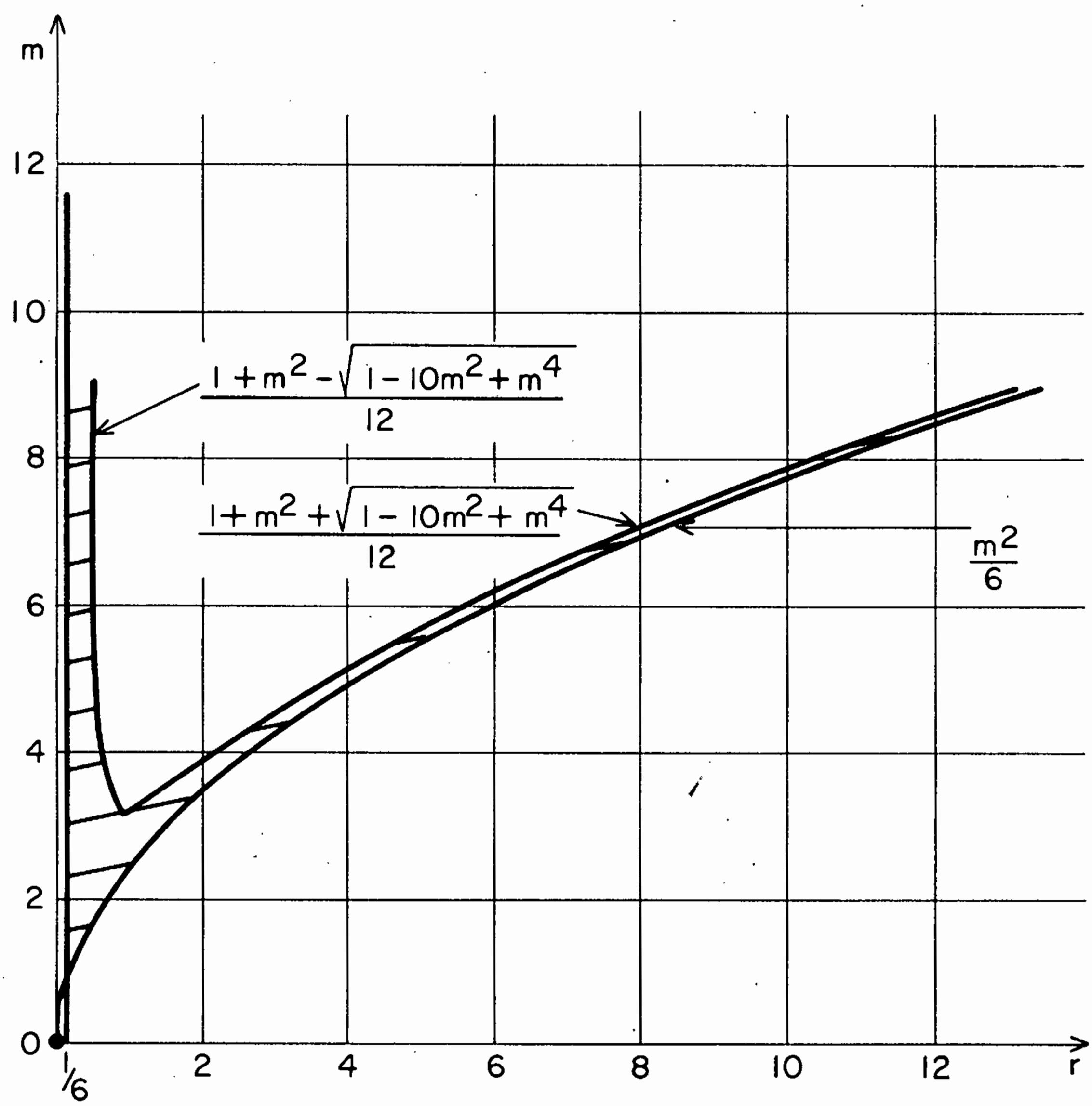

FIGURE 3

XG4-1034

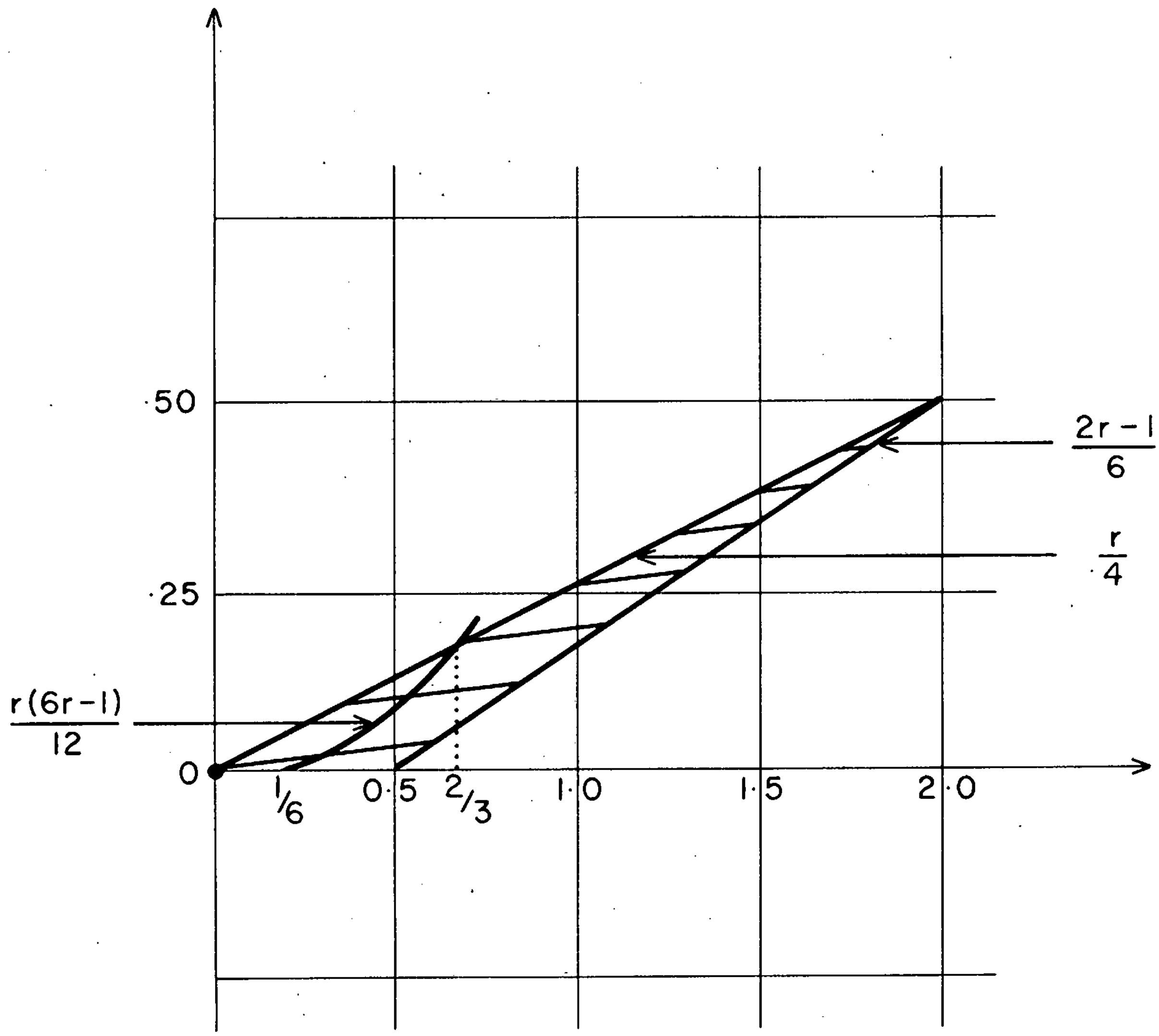

FIGURE 4

XG4-1035

$$U'_{j,k+1} = \sum_{\ell=0}^{m} a_\ell U_{j,k+\ell}, \qquad j = 1,2,\ldots\ldots,M-1,$$
$$k = 0,1,\ldots\ldots \qquad \ldots\ldots(2.13)$$

with the a_ℓ chosen such that the following relations hold:

(i) <u>for p + m uneven</u>:

$$b_p = r^p \sum_{j=0}^{\frac{m-p-1}{2}} \sum_{i=0}^{j} \left[\frac{(2j+p)!(1-2r)^{2(j-i)} r^{2i}}{\{2(j-i)\}!\ i!\ (i+p)!} a_{2j+p}\right.$$

$$\left. + \frac{(2j+p+1)!(1-2r)^{2(j-i)+1} r^{2i}}{\{2(j-i)+1\}!\ i!\ (i+p)!} a_{2j+p+1}\right] \qquad \ldots\ldots(2.14)$$

(ii) <u>for p + m even</u>:

a) <u>p < m</u>:

$$b_p = r^p \left\{ \sum_{j=0}^{\frac{m-p-2}{2}} \sum_{i=0}^{j} \left[\frac{(2j+p)!(1-2r)^{2(j-i)} r^{2i}}{\{2(j-i)\}!\ i!\ (i+p)!} a_{2j+p}\right.\right.$$

$$\left. + \frac{(2j+p+1)!(1-2r)^{2(j-i)+1} r^{2i}}{\{2(j-i)+1\}!\ i!\ (i+p)!} a_{2j+p+1}\right]$$

$$\left. + \sum_{i=0}^{\frac{m-p}{2}} \frac{m!(1-2r)^{m-p-2i} r^{2i}}{(m-p-2i)!\ i!\ (i+p)!} a_m \right\}$$

b) <u>p = m</u>:

$$b_p = r^m a_m, \qquad \ldots\ldots(2.15)$$

with the b_p, $p = 0,1,\ldots\ldots,m$, the coefficients of the difference equation (2.1), applied to these values on the time-levels $t = k\Delta t$, $t = (k+1)\Delta t$, ..., $t = (k+m)\Delta t$ according to step 2 of algorithm 1.2, results in a computational procedure which is equivalent to the difference scheme (2.1).

<u>Proof</u>:

The method of proof is the same as that used for similar theorems in chapter I.

Substitution of (1.34) into the right-hand side of (2.13) gives

$$U'_{j,k+1} = \sum_{\ell=0}^{m-1} a_\ell U_{j,k+\ell} + (1-2r)a_m U_{j,k+m-1} + r\, a_m(U_{j-1,k+m-1} + U_{j+1,k+m-1})$$

$$= \sum_{\ell=0}^{m-2} a_\ell U_{j,k+\ell}$$

$$+ [(1-4r+6r^2)\, a_m + (1-2r)\, a_{m-1} + a_{m-2}]U_{j,k+m-2}$$

$$+ [2r(1-2r)\, a_m + r\, a_{m-1}](U_{j-1,k+m-2} + U_{j+1,k+m-2})$$

$$+ r^2\, a_m\, (U_{j-2,k+m-2} + U_{j+2,k+m-2})$$

etc. Proceeding thus it can easily be seen that if p + m is uneven the coefficient of $U_{j+p,k}$ and $U_{j-p,k}$ is given by the right-hand side of (2.14). Equating the coefficients of the difference equation obtained in this way with the coefficients of (2.1) gives the relation (2.14). The relation (2.15) is obtained similarly when p + m is even.

In practice the method of algorithm 1.2 using the smoothing formula (2.13) necessitates more work for carrying out a computation than the difference equation (2.1) itself. Thus, as was remarked in connection with the methods given in chapter I, the smoothing method should be used to compute values only for those grid points on the time-level $t = (k+1)\Delta t$ for which the difference equation is not defined. Depending on whether m is comparatively large with respect to M, it might be found, however, that the simplification in programming resulting from exclusive use of the method of theorem 2.4 warrants the extra computer time used. In those cases where m is so large that the difference equation is not defined for any grid points on the time-level $t = (k+1)\Delta t$ only the method of theorem 2.4 can be used. A decision on how the difference equation (2.1) and the method of theorem 2.4 are best combined in a computation, should be made separately in each case.

The application of the method of theorem 2.4 with inclusion of values prescribed at the boundaries instead of values computed by use of the basic difference equation results in the introduction of errors. That these, however, do not have a detrimental effect on the approximate solutions obtained, can be shown in a way similar to that used in the case of theorem 1.2 (p. 22). This is substantiated by actual computations (see Table VI).

In practice the coefficients b_m, b_0 and b_1 of the difference equation (3.2) are determined first. This allows for the possibility that b_m can be chosen so as to give the smallest possible truncation error. Subsequently the a_ℓ are determined from (2.14) and (2.15).

For the computation of the results given in Table VI, an ALGOL-program was developed automatically to compute the a_ℓ, given m, r, b_m, b_1 and b_0.

A comparison of the work requirements for the method of theorem 2.4 can be made in a similar way to that used in par. 1.6 and par. 1.7. In order to do this it is assumed again that the spatial increment is kept fixed. In addition it is assumed that only the method of theorem 2.4 is used (thus no values are computed with the difference equation (2.1)). Using the maximum possible time-step in each case, the method of theorem 2.4 requires roughly $(\frac{3m+1}{2m^2})$ times as much work as the explicit difference equation (1.34).

In Table VI are given results computed by the method of theorem 2.4. The problem considered is the same as that considered in chapter I for the results given in Tables I, II, IV and V. As before $\Delta x = 0.1$ and the results given are for $x = 0.5$.

TABLE VI

t	Approx. solution using (2.13) $r = 2.0$ $m = 4$ $b_4=0.1$ $a_0=0.406\ 250$ $a_1=0.275\ 000$ $a_2=0.237\ 500$ $a_3=7.500\ 000\text{x}10^{-2}$ $a_4=6.250\ 000\text{x}10^{-3}$ $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (2.13) $r = 3.0$ $m = 5$ $b_5=0.104\ 200$ $a_0=0.456\ 250$ $a_1=0.198\ 132$ $a_2=0.246\ 564$ $a_3=8.790\ 535\text{x}10^{-2}$ $a_4=1.072\ 016\text{x}10^{-2}$ $a_5=4.288\ 066\text{x}10^{-4}$ $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (2.13) $r = 5.0$ $m = 6$ $b_6=0.128\ 600$ $a_0=0.435\ 520$ $a_1=0.223\ 412$ $a_2=0.256\ 295$ $a_3=7.555\ 507\text{x}10^{-2}$ $a_4=8.765\ 376\text{x}10^{-3}$ $a_5=4.444\ 416\text{x}10^{-4}$ $a_6=8.230\ 400\text{x}10^{-6}$ $E=0(\Delta t)+0((\Delta x)^2)$	Approx. solution using (2.13) $r = 10.0$ $m = 8$ $b_8=0.150\ 800$ $a_0=0.414\ 788$ $a_1=0.253\ 387$ $a_2=0.257\ 314$ $a_3=6.652\ 926\text{x}10^{-2}$ $a_4=7.525\ 629\text{x}10^{-3}$ $a_5=4.416\ 992\text{x}10^{-4}$ $a_6=1.403\ 646\text{x}10^{-5}$ $a_7=2.292\ 160\text{x}10^{-7}$ $a_8=1.508\ 000\text{x}10^{-9}$ $E=0(\Delta t)+0((\Delta x)^2)$
0.00	1.000 000	1.000 000	1.000 000	1.000 000
0.01				
0.02	.840 000			
0.03		.760 000		
0.04	.694 400			
0.05			.620 576	
0.06	.573 920	.576 601		
0.07				
0.08	.472 064			
0.09		.436 636		
0.10	.388 872		.390 711	.417 152
0.11				
0.12	.319 746	.329 966		
0.13				
0.14	.263 178			
0.15		.248 793	.243 799	
0.16	.216 438			
0.17				
0.18	.178 093	.187 730		
0.19				
0.20	.146 488		.153 219	.173 602

TABLE VI

t	Approx. solution using (2.13) $r = 2.0$ $m = 4$ $b_4=0.1$ $a_0=0.406\ 250$ $a_1=0.275\ 000$ $a_2=0.237\ 500$ $a_3=7.500\ 000 \times 10^{-2}$ $a_4=6.250\ 000 \times 10^{-3}$ $E=O(\Delta t)+O((\Delta x)^2)$	Approx. solution using (2.13) $r = 3.0$ $m = 5$ $b_5=0.104\ 200$ $a_0=0.456\ 250$ $a_1=0.198\ 132$ $a_2=0.246\ 564$ $a_3=8.790\ 535 \times 10^{-2}$ $a_4=1.072\ 016 \times 10^{-2}$ $a_5=4.288\ 066 \times 10^{-4}$ $E=O(\Delta t)+O((\Delta x)^2)$	Approx. solution using (2.13) $r = 5.0$ $m = 6$ $b_6=0.128\ 600$ $a_0=0.435\ 520$ $a_1=0.223\ 412$ $a_2=0.256\ 295$ $a_3=7.555\ 507 \times 10^{-2}$ $a_4=8.765\ 376 \times 10^{-3}$ $a_5=4.444\ 416 \times 10^{-4}$ $a_6=8.230\ 400 \times 10^{-6}$ $E=O(\Delta t)+O((\Delta x)^2)$	Approx. solution using (2.13) $r = 10.0$ $m = 8$ $b_8=0.150\ 800$ $a_0=0.414\ 788$ $a_1=0.253\ 387$ $a_2=0.257\ 314$ $a_3=6.652\ 926 \times 10^{-2}$ $a_4=7.525\ 629 \times 10^{-3}$ $a_5=4.416\ 992 \times 10^{-4}$ $a_6=1.403\ 646 \times 10^{-5}$ $a_7=2.292\ 160 \times 10^{-7}$ $a_8=1.508\ 000 \times 10^{-9}$ $E=O(\Delta t)+O((\Delta x)^2)$
0.00	1.000 000	1.000 000	1.000 000	1.000 000
0.01				
0.02	.840 000			
0.03		.760 000		
0.04	.694 400			
0.05			.620 576	
0.06	.573 920	.576 601		
0.07				
0.08	.472 064			
0.09		.436 636		
0.10	.388 872		.390 711	.417 152
0.11				
0.12	.319 746	.329 966		
0.13				
0.14	.263 178			
0.15		.248 793	.243 799	
0.16	.216 438			
0.17				
0.18	.178 093	.187 730		
0.19				
0.20	.146 488		.153 219	.173 602

TABLE VI

t	Analytical solution	Approx. solution using (2.13) $r = 1.0$ $m = 3$ $b_3=0.166\ 667$ $a_0=0.395\ 062$ $a_1=0.259\ 259$ $a_2=0.296\ 296$ $a_3=4.938\ 27\times10^{-2}$ $E=O((\Delta t)^2)+O((\Delta x)^4)$	Approx. solution using (2.13) $r = 2.0$ $m = 4$ $b_4=9.166\ 67\times10^{-2}$ $a_0=0.372\ 396$ $a_1=0.335\ 417$ $a_2=0.217\ 708$ $a_3=6.875\ 00\times10^{-2}$ $a_4=5.729\ 17\times10^{-3}$ $E=O((\Delta t)^2)+O((\Delta x)^4)$	Approx. solution using (2.13) $r = 3.0$ $m = 5$ $b_5=0.085\ 000$ $a_0=0.372\ 181$ $a_1=0.345\ 885$ $a_2=0.201\ 132$ $a_3=7.170\ 78\times10^{-2}$ $a_4=8.744\ 86\times10^{-3}$ $a_5=3.497\ 94\times10^{-4}$ $E=O((\Delta t)^2)+O((\Delta x)^4)$	Approx. solution using (2.13) $r = 4.0$ $m = 5$ $b_5=0.153\ 333$ $a_0=0.401\ 152$ $a_1=0.270\ 020$ $a_2=0.262\ 044$ $a_3=6.139\ 32\times10^{-2}$ $a_4=5.240\ 89\times10^{-3}$ $a_5=1.497\ 40\times10^{-4}$ $E=O((\Delta t)^2)+O((\Delta x)^4)$	Approx. solution using (2.13) $r = 5.0$ $m = 6$ $b_6=0.115\ 079$ $a_0=0.389\ 731$ $a_1=0.305\ 061$ $a_2=0.229\ 349$ $a_3=6.761\ 14\times10^{-2}$ $a_4=7.843\ 81\times10^{-3}$ $a_5=3.977\ 14\times10^{-4}$ $a_6=7.365\ 08\times10^{-6}$ $E=O((\Delta t)^2)+O((\Delta x)^4)$	Approx. solution using (2.13) $r = 10.0$ $m = 8$ $b_8=0.146\ 329$ $a_0=0.402\ 491$ $a_1=0.275\ 521$ $a_2=0.249\ 686$ $a_3=6.455\ 69\times10^{-2}$ $a_4=7.302\ 52\times10^{-3}$ $a_5=4.286\ 05\times10^{-4}$ $a_6=1.362\ 03\times10^{-5}$ $a_7=2.224\ 21\times10^{-7}$ $a_8=1.463\ 29\times10^{-9}$ $E=O((\Delta t)^2)+O((\Delta x)^4)$
0.00	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000	1.000 000
0.01	.919 331	.920 000					
0.02	.840 708	.840 772	.840 000				
0.03	.764 897	.764 587		.760 000			
0.04	.694 326	.694 417	.692 100		.680 000		
0.05	.629 614	.629 522				.618 413	
0.06	.570 664	.570 768	.572 502	.572 700			
0.07	.517 124	.517 135					
0.08	.468 561	.468 660	.467 573		.462 222		
0.09	.424 540	.424 593		.427 118			
0.10	.384 647	.384 740	.386 426			.395 306	.410 714
0.11	.348 500	.348 570					
0.12	.315 749	.315 835	.315 330	.314 483	.314 065		
0.13	.286 074	.286 149					
0.14	.259 189	.259 270	.260 341				
0.15	.234 830	.234 905		.227 800		.228 388	
0.16	.212 760	.212 836	.213 065		.213 308		
0.17	.192 764	.192 836					
0.18	.174 648	.174 719	.174 772	.233 308			
0.19	.158 234	.158 301					
0.20	.143 363	.143 428	.144 780		.144 812	.169 405	.168 670

In each case in Table VI b_m was chosen so as to conform with (2.11). In the computations only the smoothing formula was used, thus only the values $a_0, a_1, \ldots\ldots, a_m$ were needed. The value of b_m is, however, also given in each case. Note that the cases $r = 5.0$ and $r = 10.0$ have values of m that are so large that the difference equation (2.1) originally considered is not defined for any grid points on the time-level $t = (k+1)\Delta t$ as $M = 10$.

A comparison of these results with those computed by the methods given in chapter I, shows that the results of Table VI are far more accurate, especially for large values of r.

C H A P T E R III

THE APPLICATION OF THE SMOOTHING TECHNIQUE TO OBTAIN AN APPROXIMATION OF A PARABOLIC EQUATION INCORPORATING LOWER ORDER TERMS

Par. 3.1 A more general parabolic differential equation

In the previous two chapters various explicit difference methods have been discussed that can be used to compute approximate solutions of the one-dimensional diffusion equation. It was shown that, if an explicit difference equation is not defined for all grid points on the next time-level, it is possible to write such an equation as a combination of a smoothing formula and a so-called basic difference equation, which computational procedure can be defined for all grid points on the next time-level. The main advantage of this technique is that it makes possible the direct use of explicit difference approximations with better stability properties than those available at present.

The question arises of course as to whether this same technique can also be used in the case of more general parabolic equations. In order to show that this can readily be done, consider the equation

$$u_t = \sigma_0 u_{xx} + \sigma_1 u_x + \sigma_2 u \qquad \text{.....(3.1)}$$

with $0 < x < 1$, $0 < t \leq T$, σ_0, σ_1 and σ_2 constants and $\sigma_0 > 0$.

It will be assumed that appropriate initial and boundary conditions are prescribed.

Par. 3.2 A difference approximation

In order to define a difference approximation to the initial boundary value problem (3.1) the same notation and difference grid are used as in chapters I and II.

As an example of such a difference scheme which is not defined for all grid points on the time-level $t = (k+1)\Delta t$, consider the explicit equation

$$U_{j,k+1} = \sum_{p=-2}^{2} b_p \, U_{j+p,k} \quad . \qquad \ldots\ldots(3.2)$$

Due to the term $\sigma_1 u_x$ on the right-hand side of (3.1), this approximation will not be symmetric as was the case with all the approximations considered in chapters I and II. This simply means that, in general,

$$b_{-\nu} \neq b_{\nu}, \quad \nu = 1,2 \; .$$

It is assumed that the boundary and initial conditions of (3.1) are replaced by appropriate difference boundary and initial conditions.

In the case of (3.2) the following result holds:

<u>Theorem 3.1</u>

The coefficients of the difference equation (3.2):

$$U_{j,k+1} = \sum_{p=-2}^{2} b_p \, U_{j+p,k}$$

can be chosen in such a way that it is a consistent and stable approximation of the differential equation (3.1) for all
$\sigma_0 \dfrac{\Delta t}{(\Delta x)^2} \leq 2.$

<u>Proof</u>:

Using a Taylor-series expansion in the usual way, it can be shown that, under the assumption that $b_2 = b_{-2}$, the difference equation will be a consistent approximation of (3.1), if the following conditions are satisfied for $\Delta t \to 0$:

$$\begin{aligned} b_0 &= 1 - 2r + \sigma_2\Delta t + 6b_2 \\ b_1 &= r + \frac{s}{2} - 4b_2 \\ b_{-1} &= r - \frac{s}{2} - 4b_2 \end{aligned} \qquad \text{.....(3.3)}$$

with

$$r = \sigma_0 \frac{\Delta t}{(\Delta x)^2}, \qquad s = \sigma_1 \frac{\Delta t}{\Delta x}. \qquad \text{.....(3.4)}$$

The method used in chapter I to determine stability conditions, can also be used in this case. Thus the stability definition 0.2 is also used here.

The amplification factor G of (3.2) (see par. 1.4, (1.38)) can be shown to be

$$G = 1 + \sigma_2\Delta t - 4r \sin^2 \frac{\beta\Delta x}{2} + 16b_2 \sin^4 \frac{\beta\Delta x}{2} + i \sin\beta\Delta x \quad ,$$

using the relations (3.3) and the assumption that $b_2 = b_{-2}$.

Thus, writing

$$P = 1 - 4r \sin^2 \frac{\beta\Delta x}{2} + 16b_2 \sin^4 \frac{\beta\Delta x}{2}$$

and, from (3.4),

$$s = \sigma_1\sqrt{\frac{r\Delta t}{\sigma_0}} \ ,$$

$$|G| = [P^2+(2\sigma_2 P)\Delta t + \sigma_2^2(\Delta t)^2 + (\frac{r\sigma_1^2}{\sigma_0} \sin^2\beta\Delta x)\Delta t]^{\frac{1}{2}} \ . \qquad \text{.....(3.5)}$$

A necessary and sufficient condition for stability [20] is that

$$|G| \leq 1 + O(\Delta t)$$

uniformly in β . Thus stability will be obtained if

$$|P| \leq 1 .$$

This condition is the same as that for the stability of (1.35) with

$m \leq 2$, $n = 0$, $b_{0,+1} = 1$, viz.

$$\text{for} \quad 0 < r \leq 1: \quad \frac{2r-1}{8} \leq b_2 \leq \frac{r}{4}$$

$$\text{and, for} \quad 1 \leq r \leq 2: \quad \frac{r^2}{8} \leq b_2 \leq \frac{r}{4} \; , \qquad \text{.....(3.6)}$$

(see Fig. 2 and corollary 1.2) which proves the theorem.

In the case of the difference equation (3.2), with the conditions (3.3), the truncation error is given by

$$E = O(\Delta t) + O(\Delta x) \quad . \qquad \text{.....(3.7)}$$

Thus the stability conditions for the difference equation (3.2) are not influenced by $\sigma_1 \neq 0$, $\sigma_2 \neq 0$. On the other hand the truncation error is increased if $\sigma_1 \neq 0$.

Par. 3.3 A smoothing formula

The difference equation (3.2) is not defined for all grid points on the time-level $t = (k+1)\Delta t$. As before, this equation can however be written as a combination of a suitable basic difference equation and a smoothing formula, which results in a computational procedure defined for all grid points on the time-level $t = (k+1)\Delta t$.

One difference approximation that can be used as basic equation is:

$$U_{j,k+1} = \sum_{p=-1}^{1} \hat{b}_p U_{j+p,k} \qquad \text{.....(3.8)}$$

with

$$\begin{aligned} \hat{b}_0 &= 1 - 2r + \sigma_2 \Delta t \\ \hat{b}_1 &= \quad r + \frac{s}{2} \\ \hat{b}_{-1} &= \quad r - \frac{s}{2} \; , \end{aligned} \qquad \text{.....(3.9)}$$

r and s as in (3.4).

One possible way of combining a smoothing formula with this basic difference equation is to use algorithm 1.2 with $\hat{n}_2 = 1$ and (3.9) instead of (1.34).

A smoothing formula that can be used in step 2 of this algorithm is:

Theorem 3.2

Given an approximate solution of the differential equation (3.1) for $t = k\Delta t$ and values for $t = (k+1)\Delta t$ computed with (3.9) according to step 1 of algorithm 1.2 with $\hat{n}_2 = 1$, then the smoothing formula (1.58) with $\hat{n}_2 = \hat{m} = 1$, $\hat{n}_1 := 0$:

$$U'_{j,k+1} = a_{0,0}\, U_{j,k} + a_{-1,0}\, U_{j-1,k} + a_{1,0}\, U_{j+1,k} + a_{-1,1} U_{j-1,k+1} + a_{1,1}\, U_{j+1,k+1} \qquad \ldots..(3.10)$$

with

$$a_{0,0} = b_0 - 2\left(\frac{4r^2+s^2}{4r^2-s^2}\right) b_2$$

$$a_{-1,0} = b_{-1} - 2\left(\frac{1-2r+\sigma_2\Delta t}{2r - s}\right) b_2$$

$$a_{1,0} = b_1 - 2\left(\frac{1-2r+\sigma_2\Delta t}{2r + s}\right) b_2$$

$$a_{-1,1} = \left(\frac{2}{2r-s}\right) b_2$$

$$a_{1,1} = \left(\frac{2}{2r+s}\right) b_2 , \qquad \ldots..(3.11)$$

the b_p, $p = 0, \pm 1, 2$, being the coefficients of the difference equation (3.2):

$$U_{j,k+1} = \sum_{p=-2}^{2} b_p\, U_{j+p,k} ,$$

applied to these values on the time-levels $t = k\Delta t$, $t = (k+1)\Delta t$ according to step 2 of algorithm 1.2, results in a computational procedure which is equivalent to the difference scheme (3.2).

Proof:

Substituting (3.8) into the right-hand side of (3.10) gives the difference equation

$$U'_{j,k+1} = (a_{0,0}+a_{-1,1}\hat{b}_1+a_{1,1}\hat{b}_{-1})\, U_{j,k}$$

$$+(a_{-1,0}+a_{-1,1}\hat{b}_0)U_{j-1,k} + (a_{1,0}+a_{1,1}\hat{b}_0)\, U_{j+1,k}$$

$$+ a_{-1,1}\hat{b}_{-1}\, U_{j-2,k} + a_{1,1}\hat{b}_1\, U_{j+2,k} \,.$$

Equating the coefficients of this difference equation with those of (3.2) gives the relations

$$\begin{aligned}
b_0 &= a_{0,0} + \hat{b}_1 a_{-1,1} + \hat{b}_{-1} a_{1,1} \\
b_{-1} &= a_{-1,0} + \hat{b}_0 a_{-1,1} \\
b_1 &= a_{1,0} + \hat{b}_0 a_{1,1} \\
b_{-2} &= \hat{b}_{-1} a_{-1,1} \\
b_2 &= \hat{b}_1 a_{1,1}
\end{aligned}$$

with the b_p, $p = 0,\pm1,\pm2$, the coefficients of (3.2). Solving for the $a_{i,\ell}$ and using the relations (3.9) gives (3.11).

As was found with all the smoothing formulas given in chapter I, more work is necessary to carry out a computation with the basic difference equation (3.8), (3.9) combined with the smoothing formula (3.10), (3.11) than that required when the difference equation (3.2) is used to perform the same computation. On the other hand the computational procedure described in theorem 3.2 is defined for all grid points on the time-level $t = (k+1)\Delta t$. Thus, by using the procedure of theorem 3.2, for example, to compute the values $U_{1,k+1}$ and $U_{M-1,k+1}$ and (3.2) to compute $U_{j,k+1}$, $j = 2,3,\ldots\ldots,M-2$, it is possible to make practical use of (3.2) with a minimum increase in the work necessary.

CHAPTER IV

THE EXTENSION OF THE SMOOTHING TECHNIQUE TO MORE-DIMENSIONAL PROBLEMS

Par. 4.1 More-dimensional diffusion problems

The smoothing technique described in previous chapters can also be extended to more-dimensional problems. In order to simplify the formulas, a two-dimensional problem will be treated as an example. The extension of the results to n dimensions can be effected in an obvious way. (In most cases this requires merely that 2 be replaced by n).

Consider the diffusion equation

$$u_t = \sigma_1 u_{x_1 x_1} + \sigma_2 u_{x_2 x_2} \qquad \ldots\ldots(4.1)$$

with $0 < t \leq T$, $0 < x_\nu < 1$, $\sigma_\nu > 0$, $\nu = 1,2$. It will be assumed that initial and boundary conditions are prescribed. (See, for example, [1]).

Par. 4.2 An explicit difference approximation

In order to construct a difference equation that can be used to compute an approximate solution of (4.1), a rectangular difference grid is defined over the cylinder over which (4.1) is defined. The mesh-widths along the spatial co-ordinate axes are indicated by Δx_ν, $\nu = 1,2$, and along the t-axis (as usual) by $\Delta t > 0$. The co-ordinates of the grid points are given by $(j_1 \Delta x_1, j_2 \Delta x_2, k\Delta t)$, j_ν, $\nu = 1,2$, and k non-negative integers.

Consider the following explicit difference equation:

$$U_{j_1,j_2,k+1} = \sum_{p=-2}^{2} [b_p^{(1)} U_{j_1+p,j_2,k} + b_p^{(2)} U_{j_1,j_2+p,k}]. \qquad \ldots\ldots(4.2)$$

It will be assumed that

$$b_p^{(\nu)} = b_{-p}^{(\nu)}, \quad p = 1,2; \quad \nu = 1,2 . \qquad \ldots\ldots(4.3)$$

In addition it will be assumed that the prescribed initial and boundary conditions are replaced by appropriate conditions.

If (4.2) is to be considered an approximation of (4.1), consistency and stability have to be ensured. Using Taylor-series expansions of the terms in (4.2) and comparing with (4.1), the following consistency conditions are obtained, viz. that the coefficients of (4.2) must satisfy the relations

$$\sum_{\nu=1}^{2} \sum_{p=-2}^{2} b_p^{(\nu)} = 1,$$

$$b_1^{(\nu)} + 4\, b_2^{(\nu)} = r_\nu, \qquad \nu = 1,2, \qquad \text{.....(4.4)}$$

in the limit with $\Delta t \to 0$. Here

$$r_\nu = \frac{\sigma_\nu \Delta t}{(\Delta x_\nu)^2}, \qquad \nu = 1,2 . \qquad \text{.....(4.5)}$$

The truncation error is given by

$$E = 0(\Delta t) + 0((\Delta x_1)^2) + 0((\Delta x_2)^2) . \qquad \text{.....(4.6)}$$

The method used to derive stability conditions with respect to the stability definition 0.2 in the 1-dimensional case (chapter I) can also be used in the above case. Thus, using (4.4) and the fact that the problem considered is linear, and substituting into (4.2) one term of a Fourier-series expansion of the solution of the difference equation, it follows that a necessary and sufficient condition for stability is that the modulus of the amplification factor:

$$|G| = |1 - 4r_1\eta_1 - 4r_2\eta_2 + 16b_2^{(1)}x_1^2 + 16b_2^{(2)}x_2^2| \leq 1 , \qquad \text{.....(4.7)}$$

with

$$\eta_\nu = \sin^2 \left(\frac{\beta_\nu \Delta x_\nu}{2}\right), \qquad \nu = 1,2,$$

and β_ν real and arbitrary.

As the η_ν are independent of each other, (4.7) will hold if

$$\left|\frac{1}{2} - 4r_\nu\eta_\nu + 16b_2^{(\nu)}\eta_\nu^2\right| \leq \frac{1}{2}, \quad \nu = 1,2,$$

as allowance has to be made for all possible choices of the β_ν. This condition will be satisfied if, for

$$\text{i)} \quad 0 < r_\nu \leq \frac{1}{2} : \qquad \frac{4r_\nu-1}{16} \leq b_2^{(\nu)} \leq \frac{r_\nu}{4}, \quad \nu = 1,2,$$

whereas, for

$$\text{ii)} \quad \frac{1}{2} \leq r_\nu \leq 1 : \qquad \frac{r_\nu^2}{4} \leq b_2^{(\nu)} \leq \frac{r_\nu}{4}, \quad \nu = 1,2 . \qquad \text{.....(4.8)}$$

(Compare (4.8) with (1.51)).

Par. 4.3 <u>A smoothing formula</u>

As in the case of difference equations with $m \geq 2$ used to approximate the one-dimensional diffusion equation in chapters I and II, it follows that the difference equation (4.2) is not defined for all grid points on the time-level $t = (k+1)\Delta t$. As before, however, this difference equation can be expressed as a combination of a suitable basic difference equation and smoothing formula. By appropriate choice of the basic difference equation and smoothing formula, this procedure can be defined for all grid points on the time-level $t = (k+1)\Delta t$, excluding of course the boundary grid points.

An example of such a basic difference equation and smoothing formula is given here. As was shown before, these are not unique.

As the basic difference equation the most simple explicit two-level approximation to (4.1) will be used:

$$U_{j_1,j_2,k+1} = (1-2r_1-2r_2)\,U_{j_1,j_2,k} + r_1(U_{j_1-1,j_2,k} + U_{j_1+1,j_2,k}) + r_2(U_{j_1,j_2-1,k} + U_{j_1,j_2+1,k}) \,. \qquad \text{..... (4.9)}$$

This approximation is consistent with the differential equation (4.1). From the stability conditions (4.8) it follows that, as $b_2^{(\nu)} = 0$, $\nu = 1,2$, (4.9) will be stable for all

$$0 < r_\nu \leq \frac{1}{4} , \quad \nu = 1,2 . \qquad \ldots\ldots(4.10)$$

In the definition of the difference approximation (4.2) it was assumed that the initial and boundary conditions of the initial boundary value problem (4.1) have been replaced by appropriate conditions. These same conditions can be used to define the initial and boundary values in the case of (4.9).

In chapter I it was assumed that Δx has been so chosen that $M\Delta x = 1$. In analogy with this, it is assumed here that $M_\nu \Delta x_\nu = 1$, $\nu = 1,2$.

The difference equation (4.9) can now be used as basic equation in the following algorithm (compare algorithm 1.2):

<u>Algorithm 4.1</u>

Step 1: Using (4.9) the values $U_{j_1,j_2,1}$, $j_1 = 1,2,\ldots\ldots,M_1-1$, $j_2 = 1,2,\ldots\ldots,M_2-1$, are computed from the known values $U_{j_1,j_2,0}$, $j_1 = 0,1,\ldots\ldots,M_1$, $j_2 = 0,1,\ldots\ldots,M_2$, given by the conditions that replace the initial and boundary values of (4.1) in the definition of (4.9).

Step 2: To these known and computed values on the time-levels $t = 0$, $t = \Delta t$ a smoothing formula is applied to give values $U'_{j_1,j_2,1}$, $j_1 = 1,2,\ldots\ldots,M_1-1$, $j_2 = 1,2,\ldots\ldots,M_2-1$.

It is required that these smoothed values should be good approximations of the solution of the initial boundary value problem (4.1).

Step 3: Using these smoothed values for the time-level $t = \Delta t$, step 1 is repeated to give values for $t = 2\Delta t$. With these values step 2 is repeated to give smoothed values $U'_{j_1,j_2,2}$. This process can now be repeated for any desired number of cycles.

In this algorithm the following smoothing formula can be used:

<u>Theorem 4.8</u>

Given an approximate solution of the initial boundary value problem (4.1) for the time-level $t = k\Delta t$ and values for the time-level $t = (k+1)\Delta t$ computed according to step 1 of algorithm 4.1, then the smoothing formula:

$$U'_{j_1,j_2,k+1} = \sum_{\ell=0}^{1} [a_{0,0,\ell}\, U_{j_1,j_2,k+\ell} + a_{1,0,\ell}\,(U_{j_1-1,j_2,k+\ell} + U_{j_1+1,j_2,k+\ell}) + a_{0,1,\ell}\,(U_{j_1,j_2-1,k+\ell} + U_{j_1,j_2+1,k+\ell})] + \sum_{\substack{i_1=-1 \\ i_1\neq 0}}^{1} \sum_{\substack{i_2=-1 \\ i_2\neq 0}}^{1} a_{i_1,i_2,0}\, U_{j_1+i_1,j_2+i_2,k} \quad \ldots\ldots(4.11)$$

with

$$a_{0,0,0} = (1 - 2r_1 - 2r_2) + 4b_2^{(1)} + 4b_2^{(2)}$$

$$a_{1,0,0} = r_1 - \left(\frac{1+2r_1-2r_2}{r_1}\right) b_2^{(1)}$$

$$a_{0,1,0} = r_2 - \left(\frac{1-2r_1+2r_2}{r_2}\right) b_2^{(2)}$$

$$a_{1,1,0} = a_{-1,1,0} = a_{1,-1,0} = a_{-1,-1,0} = -\left(\frac{r_2}{r_1}\, b_2^{(1)} + \frac{r_1}{r_2}\, b_2^{(2)}\right)$$

$$a_{0,0,1} = 0$$

$$a_{1,0,1} = \frac{1}{r_1}\, b_2^{(1)}$$

$$a_{0,1,1} = \frac{1}{r_2}\, b_2^{(2)}$$

with $b_2^{(1)}$ and $b_2^{(2)}$ the coefficients of the difference equation (4.2), applied to these values on the time-levels $t = k\Delta t$, $t = (k+1)\Delta t$ according to step 2 of algorithm 4.1, results in a computational procedure which is equivalent to the difference scheme 4.2

Proof:

In accordance with step 1 substitute (4.9) into the right-hand side of (4.11) to give only values defined on the time-level $t = k\Delta t$, viz.

$$
\begin{aligned}
U'_{j_1,j_2,k+1} = {} & [a_{0,0,0}+(1-2r_1-2r_2)a_{0,0,1}+2r_1a_{1,0,1}+2r_2a_{0,1,1}]U_{j_1,j_2,k} \\
& + [a_{1,0,0}+ r_1a_{0,0,1} +(1-2r_1-2r_2)a_{1,0,1}](U_{j_1-1,j_2,k}+U_{j_1+1,j_2,k}) \\
& + [a_{0,1,0}+ r_2a_{0,0,1} +(1-2r_1-2r_2)a_{0,1,1}](U_{j_1,j_2-1,k}+U_{j_1,j_2+1,k}) \\
& + r_1\, a_{1,0,1}\, (U_{j_1-2,j_2,k} + U_{j_1+2,j_2,k}) \\
& + r_2\, a_{0,1,1}\, (U_{j_1,j_2-2,k} + U_{j_1,j_2+2,k}) \\
& + [a_{1,1,0} + r_1\, a_{0,1,1} + r_2\, a_{1,0,1}]\, U_{j_1+1,j_2+1,k} \\
& + [a_{-1,1,0}+ r_1\, a_{0,1,1} + r_2\, a_{1,0,1}]\, U_{j_1-1,j_2+1,k} \\
& + [a_{1,-1,0}+ r_1\, a_{0,1,1} + r_2\, a_{1,0,1}]\, U_{j_1+1,j_2-1,k} \\
& + [a_{-1,-1,0}+r_1\, a_{0,1,1} + r_2\, a_{1,0,1}]\, U_{j_1-1,j_2-1,k} \;.
\end{aligned}
$$

Equating the coefficients of this difference equation with those of (4.2) gives:

$$
\begin{aligned}
b_0^{(1)} + b_0^{(2)} &= a_{0,0,0} + (1-2r_1-2r_2)a_{0,0,1} + 2r_1a_{1,0,1} + 2r_2\, a_{0,1,1} \\
b_1^{(1)} &= a_{1,0,0} + r_1\, a_{0,0,1} + (1-2r_1-2r_2)\, a_{1,0,1} \\
b_1^{(2)} &= a_{0,1,0} + r_2\, a_{0,0,1} + (1-2r_1-2r_2)\, a_{0,1,1} \\
b_2^{(1)} &= r_1\, a_{1,0,1} \\
b_2^{(2)} &= r_2\, a_{0,1,1}
\end{aligned}
$$

$$0 = a_{1,1,0} + r_1 a_{0,1,1} + r_2 a_{1,0,1}$$

$$0 = a_{-1,1,0} + r_1 a_{0,1,1} + r_2 a_{1,0,1}$$

$$0 = a_{1,-1,0} + r_1 a_{0,1,1} + r_2 a_{1,0,1}$$

$$0 = a_{-1,-1,0} + r_1 a_{0,1,1} + r_2 a_{1,0,1} .$$

Using the relations (4.4), the relations (4.12) are obtained directly from these equations.

As is the case with all the smoothing procedures given in the preceding chapters, a computation by the method of theorem 4.1 requires more work than necessary to obtain the same result with (4.2). Thus, as was previously suggested, the procedure of theorem 4.1 – which is defined for all grid points on the time-level $t = (k+1)\Delta t$ – should be used to compute approximate solutions only for those grid points on the next time-level for which (4.2) is not defined. The remaining values can then be computed directly with (4.2).

It can, in the case of theorem 4.1, also be shown that there will be no detrimental effect on the overall approximation error obtained if the boundary values are replaced by values computed from the prescribed values rather than values computed with (4.9).

REFERENCES

[1] BIRTWISTLE, G.M.: The explicit solution of the equation of heat conduction, Computer Journal, Vol.11, No. 3, 1968, p. 317.

[2] CARSLAW, H.S. and JAEGER, J.C.: Conduction of Heat in Solids, The Clarendon Press, Oxford, 1947.

[3] COLLATZ, L.: Numerische Behandlung von Differentialgleichungen, Springer-Verlag, Berlin, 1951.

[4] DOUGLAS, J. and GUNN, J.: A general formulation of alternating direction methods, I, Numerische Mathematik, Vol. 6, 1964, p. 428.

[5] DU FORT, E.C. and FRANKEL, S.P.: Stability conditions in the numerical treatment of parabolic differential equations, Mathematical Tables and Other Aids to Computation, Vol. 7, 1953, p. 135.

[6] DURAND, E.: Solutions Numériques des Équations Algébriques, Tome I et II, Masson et Cie., Paris, 1960/1.

[7] FORSYTHE, G.E. and WASOW, W.R.: Finite-Difference Methods for Partial Differential Equations, John Wiley and Sons, Inc., New York, 1960.

[8] GANTMACHER, F.R.: Applications of the Theory of Matrices, Interscience Publishers, Inc., New York, 1959

[9] GODUNOV, S.K. and RYABENKI, V.S.: The Theory of Difference Schemes, North-Holland Publishing Co., Amsterdam, 1964.

[10] GORDON, P.: Nonsymmetric difference equations, Journal of the Society for Industrial and Applied Mathematics, Vol. 13, 1965, p. 667.

[11] HILDEBRAND, F.B.: Finite-Difference Equations and Simulations, Prentice-Hall Inc., Englewood Cliffs, N.J., 1968.

[12] JOHN, F.: On the integration of parabolic equations by difference methods, Communications on Pure and Applied Mathematics, Vol. 5, 1955, p. 155.

[13] KREISS, H.O.: Über die Stabilitätsdefinition für Differenzengleichungen die partielle Differentialgleichungen approximieren, BIT Nordisk Tidskrift for Informationsbehandling, Vol. 2, 1962, p. 153.

[14] LAX, P.D. and RICHTMYER, R.D.: Survey of the stability of linear finite difference equations, Communications on Pure and Applied Mathematics, Vol. 9, 1956, p. 267.

[15] MILNE, W.E.: Numerical Solution of Differential Equations, John Wiley and Sons, Inc., London, 1953.

[16] OBRESCHKOFF, N.: Verteilung und Berechung der Nullstellen Reeller Polynome, Deutscher Verlag der Wissenschaften, Berlin, 1963.

[17] O'BRIEN, G.G., HYMAN, M.A. and KAPLAN, S.: A study of the numerical solution of partial differential equations, Journal of Mathematics and Physics, Vol.29, 1951, p.223.

[18] PEACEMAN, D.W. and RACHFORD, H.H. Jr.: The numerical solution of parabolic and elliptic differential equations, Journal of the Society for Industrial and Applied Mathematics, Vol.3, 1955, p.28.

[19] RICHARDSON, L.F.: The approximate arithmetical solution by finite differences of physical problems involving differential equations with an application to the stresses in a masonry dam, Philosophical Transactions of the Royal Society of London, Series A, Vol. 210, p. 307.

[20] RICHTMYER, R.D. and MORTON, K.W.: Difference Methods for Initial-Value Problems, 2nd Edition, Interscience Publishers, New York, 1967.

[21] RJABENKI, V.S. and FILLIPOW, A.F.: Über die Stabilität von Differenzengleichungen, Deutscher Verlag der Wissenschaften, Berlin, 1960.

[22] SAUL'YEV, V.K.: On a method of numerical integration of a diffusion equation, Doklady Akademia Nauk SSSR, Vol. 115, No. 6, 1957, p. 1077.

[23] SAUL'YEV, V.K.: On the question of the numerical integration of parabolic equations, Doklady Akademia Nauk SSSR, Vol. 117, No. 4, 1957, p. 36.

[24] SAUL'YEV, V.K.: Integration of Equations of Parabolic Type by the Method of Nets, Pergamon Press, Oxford, 1964.

[25] SCHMEIDLER, W.: Vorträge über Determinanten und Matrizen mit Anwendungen in Physik und Technik, Akademie-Verlag, Berlin, 1949.

[26] VAN DER HOUWEN, P.J.: Finite Difference Methods for Solving Partial Differential Equations, Mathematisch Centrum, Amsterdam, 1968.