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On the Accuracy of Implicit Difference Approximations to the Equation of Heat Flow

By Wolfgang Wasow

1. Introduction. Implicit finite difference methods are gaining favor in the numerical solution of initial value problems for partial differential equations, because their computational stability is comparatively insensitive to the mesh ratios. The difference equation problems of importance in the applications are mostly too complicated to permit a theoretical analysis of their approximating qualities. It is a reasonable working hypothesis that the properties of the simplest linear difference equations with constant coefficients are indicative of the situation to be expected in many more involved problems.

The present paper is devoted to a study of the convergence, the stability and the truncation error of implicit difference approximations to the initial value problem defined by the differential equation

$$(1.1) \quad L[u] \equiv u_t - u_{xx} = 0, \quad 0 < x < \pi, \quad 0 < t \leq T,$$

where the subscripts indicate partial differentiations, and the subsidiary conditions

$$(1.2) \quad u(x, 0) = f(x), \quad u(0, t) = u(\pi, t) = 0,$$

in which $f(x)$ is a given function. The approximating difference equation to be considered is

$$(1.3) \quad L_{h,k}[U] \equiv k^{-1}\{U(x, t+k) - U(x, t)\} - sh^{-2}\{U(x+h, t+k) - 2U(x, t+k) + U(x-h, t+k)\} - (1-s)h^{-2}\{U(x+h, t) - 2U(x, t) + U(x-h, t)\} = 0, \quad 0 < x < \pi, \quad 0 < t \leq T.$$

The function $U(x, t)$ must also satisfy the same subsidiary conditions as $u(x, t)$, i.e.,

$$(1.4) \quad U(x, 0) = f(x), \quad U(0, t) = U(\pi, t) = 0.$$

It will be assumed throughout that π/h is an integer. Furthermore, h and k will be restricted to intervals $0 < h \leq h_1 < 1$, $0 < k \leq k_1 < 1$.

The cases $s = 0$, $s = 1$ have been extensively studied in the literature (See, e.g., [1], [2], [3]). A paper in process of publication by M. L. Juncosa and D. Young [4] contains an appraisal of the truncation error for $s = \frac{1}{2}$. This appraisal is less sharp than the one contained in theorem 2 of the present paper. P. Lax and R. Richtmyer [5] have applied their general theory of finite difference approximations for initial value problems to an equation slightly more general than (1.3).

Their arguments are based on the norm $\left\{ \int_0^\pi \phi^2(x, t) dx \right\}^{\frac{1}{2}}$. The elegant methods by means of which they study the convergence and stability can doubtless be extended to yield appraisals of the truncation error as well, but since uniform or pointwise appraisals are more satisfactory to the numerical analyst than bounds on the mean square norm, it is hoped that the results of the present paper are of some interest.

2. The Convergence of $U(x, t)$. If $f(x)$ is integrable and $\sum_{r=1}^\infty b_r \sin rx$ is its Fourier sine-series the function

$$(2.1) \quad u(x, t) = \sum_{r=1}^\infty \exp(-r^2 t) b_r \sin rx$$

is, for $t > 0$, a solution of the differential equation (1.1), as can be readily verified. Under rather mild additional conditions on $f(x)$ this function fulfills also the boundary conditions (1.2), at least in some weak sense [3]. Here, the stronger hypothesis

$$(2.2) \quad \sum_{r=1}^\infty |b_r| < \infty$$

will be made, which is, for instance, satisfied if

$$(2.3) \quad f(0) = f(\pi) = 0,$$

and $f(x)$ is continuous and has a piecewise continuous derivative.

The method of separation of variables leads to the formal trigonometric series

$$(2.4) \quad U(x, t) \sim \sum_{r=1}^\infty E_r t^{1/k} b_r \sin rx$$

for the solution of (1.3) and (1.4). Here E_r is defined by

$$(2.5) \quad E_r = \frac{h^2 - 4(1-s)k \sin^2(rh/2)}{h^2 + 4sk \sin^2(rh/2)}.$$

The derivation of (2.4) is straightforward and will be omitted.

If

$$(2.6) \quad 2(1 - 2s)k - h^2 \leq 0,$$

and only then, it follows that

$$(2.7) \quad |E_r| \leq 1,$$

for all r . In this case the series in (2.4) is uniformly convergent, thanks to condition (2.2), and represents therefore the solution of the difference problem.

In order to prove the convergence of $U(x, t)$ to $u(x, t)$ it will now be shown that

$$(2.8) \quad \lim_{h, k \rightarrow 0} E_r^{t/k} = \exp(-r^2 t).$$

If k is so small that $|kr^2(1-s)| < 1$ and $|kr^2s| < 1$, it follows from part a) of the Lemma in section 5 that

$$|\log E_r + 4h^{-2}k \sin^2(rh/2)| \leq c(4h^{-2}k \sin^2(rh/2))^2, \quad c \text{ a constant.}$$

The right member is a bounded function of h , and it can therefore be concluded from this inequality that

$$\lim_{k \rightarrow 0} (t/k) (\log E_r + 4h^{-2}k \sin^2(rh/2)) = 0,$$

uniformly in h . Hence,

$$(2.9) \quad \lim_{k \rightarrow 0} E_r^{t/k} = \exp\{-4h^{-2}t \sin^2(rh/2)\},$$

and (2.8) is now obtained by letting h tend to zero.

Since, under the hypotheses made, the series (2.4) converges uniformly, for all small h and k , the passage to the limit indicated by (2.8) can be performed termwise and leads to the series (2.1). Thus the following theorem has been proved.

THEOREM 1. *If the Fourier sine coefficients b_r of $f(x)$ satisfy the condition*

$$\sum_{r=1}^{\infty} |b_r| < \infty,$$

and if h and k tend to zero in such a way that $2(1-2s)k - h^2 \leq 0$ then

$$\lim_{h, k \rightarrow 0} U(x, t) = u(x, t),$$

where U and u solve the problems (1.3), (1.4), and (1.1), (1.2), respectively.

For $s < \frac{1}{2}$, the inequality (2.6) restricts the size of the ratio k/h^2 . For $s \geq \frac{1}{2}$ theorem 1 proves the convergence of U to u for any form of the passage to the limit $h \rightarrow 0, k \rightarrow 0$. This goes beyond the frequently made statement that k/h^2 may have any constant value in this case. Observe that s is not restricted to the interval $0 \leq s \leq 1$.

COROLLARY. *Denote by $u_h(x, t)$ the solution of the difference-differential equation problem obtained from (1.3) by substituting U_t for $k^{-1}\{U(x, t+k) - U(x, t)\}$ and by imposing the subsidiary conditions (1.4). Then*

$$\lim_{k \rightarrow 0} U(x, t) = u_h(x, t),$$

provided (2.2) is true.

To prove this corollary it suffices to refer to (2.9) and to show that the uniformly convergent series obtained from (2.4) by substituting $\exp\{-4h^{-2}t \sin^2(rh/2)\}$ for

E_r satisfies the difference-differential equation and the boundary conditions (1.4). This can be done by simple verification. The condition (2.6) is, of course, true for all sufficiently small k , if h is kept fixed.

It is easily seen that an analogous corollary could be stated concerning the difference-differential equation obtained if the difference quotients with respect to x in (1.3) are replaced by the corresponding derivatives. Here, however, the condition $s \geq \frac{1}{2}$ has to be imposed in order to maintain the inequality (2.6). The solution of this problem is the series obtained from (2.4) by substituting

$$\frac{1 - (1 - s)kr^2}{1 + skr^2}$$

for E_r .

Such difference-differential equations are sometimes used on analog machines. The arguments of this section justify these procedures mathematically.

3. The Truncation Error. In this section the order of magnitude of the truncation error $U - u$ will be determined (see theorem 2 below). The condition (2.6) is known to be necessary at least for $s = 0$, if convergence for all reasonably regular initial functions $f(x)$ is desired. Very likely it is necessary for all $0 < s < \frac{1}{2}$. Various heuristic arguments lead to the conjecture that $s = \frac{1}{2}$ is the most favorable choice as far as the order of magnitude of the truncation error is concerned. For instance, if $L_{h,k}[u]$ in (1.3) is developed in powers of h and k , where u is a solution of (1.1), the resulting series begins with terms of order $O(k + h^2)$, except if $s = \frac{1}{2}$, in which case the leading terms are $O(k^2 + h^2)$. The results of this section will confirm the expected exceptional role of the value $s = \frac{1}{2}$. Since the purpose of implicit methods is to gain more freedom in the choice of h and k , the range $0 < s < \frac{1}{2}$, in which the condition (2.6) is necessary, is of little interest. Throughout this section the inequalities

$$(3.1) \quad \frac{1}{2} \leq s \leq 1$$

will therefore be imposed.

In view of theorem 1 the convergence of U to u takes place no matter how h and k tend to zero, if (3.1) is true. However, the order of magnitude of $U - u$ is very likely affected if h is exponentially small with respect to k . Here the inequality

$$(3.2) \quad h/k \geq p > 0, \quad p \text{ a constant}$$

will be assumed to be true. Without too much complication the arguments apply also to the more general case that $h^\beta/k \geq p > 0$, $\beta > 0$. The restriction to (3.2) is motivated by the desire to avoid involved formulas. The condition (3.2) is considerably weaker than the hypothesis $k/h^2 = \text{const}$ frequently met in this connection. It is also milder than the assumption $k = O(h/\log h)$ made in [4].

Finally, the conditions on $f(x)$ must be tightened in this section. It will be assumed that

$$(3.3) \quad |b_r| \leq Kr^{-3}.$$

This is, for instance, the case if (2.3) is true and $f(x)$ possesses an integrable third

derivative in $0 \leq x \leq \pi$, for three integrations by parts show that then

$$(3.4) \quad b_r = \frac{2}{\pi} \int_0^\pi f(x) \sin rx dx = \frac{2}{\pi} r^{-3} [(-1)^r f''(\pi) - f''(0)] \\ - \frac{2}{\pi} r^{-3} \int_0^\pi f'''(x) \cos rx dx.$$

The following theorem will now be proved.

THEOREM 2. Let $\frac{1}{2} \leq s \leq 1$, $h/k \geq p > 0$, $k \leq t \leq T$, $h \leq h_1 < p/2$. Assume that $f(x)$ possesses an absolutely integrable bounded third derivative and that $f(0) = f(\pi) = 0$. Then

$$|U(x, t) - u(x, t)| \leq ct^{-1}(h^2 + k^\alpha),$$

where $\alpha = 1$ for $s \neq \frac{1}{2}$, and $\alpha = 2$ for $s = \frac{1}{2}$. Also,

$$c = M \sup_{0 \leq x \leq \pi} (|f''(x)| + |f'''(x)|).$$

The constant M depends on s , p and T only.

The truncation error will be appraised by splitting the series in

$$(3.5) \quad U(x, t) - u(x, t) = \sum_{r=1}^{\infty} (E_r^{t/k} - \exp(-r^2 t)) b_r \sin rx$$

into four parts V_1, V_2, V_3, V_4 corresponding, respectively, to the ranges $r \leq r_1$, $r_1 < r \leq r_2$, $r_2 < r \leq r_3$, $r_3 < r$. The integers $r_j, j = 1, \dots, 4$, are defined below.

a) The range $r \leq r_1$. The numerator

$$h^2 - 4(1-s)k \sin^2(rh/2)$$

of E_r vanishes if

$$(3.6) \quad r = 2/h \arcsin \frac{h}{2\sqrt{(1-s)k}}.$$

Let r_0 be the smallest positive determination of the right member of (3.6) if the latter is real, i.e., if $h/(2\sqrt{(1-s)k}) \leq 1$. Otherwise, set $r_0 = \infty$. If r_0 is finite it lies in the interval

$$(3.7) \quad \frac{1}{\sqrt{(1-s)k}} \leq r_0 \leq \pi/2 \frac{1}{\sqrt{(1-s)k}},$$

because $1 \leq (\arcsin q)/q \leq \pi/2$, for $0 \leq q \leq 1$, if the principal value of $\arcsin q$ is taken. Define r_1 by

$$(3.8) \quad r_1 = [\sqrt{\theta p/h}], \quad 0 < \theta < 1.$$

Here $[z]$ designates the largest integer not exceeding z .

The letters $c_j, j = 1, 2, \dots$, below denote positive constants that may depend on s, p , and T , but not on h, k, x, t , or $f(x)$.

In order to appraise V_1 let $r \leq r_1$, and observe that, by (3.2), (3.7) and (3.8),

$$(3.9) \quad r_1 \leq r_0/\sqrt{2}.$$

Also, if z_r is defined by

$$(3.10) \quad z_r = 4kh^{-2} \sin^2 (rh/2),$$

it follows from (3.8) that

$$(3.11) \quad z_r \leq kr_1^2 \leq \theta, \quad \text{for } r \leq r_1.$$

Since

$$E_r = \frac{1 - (1 - s)z_r}{1 + sz_r},$$

an application of the Lemma of section 5 shows that

$$(3.12) \quad E_r^{t/k} = \exp [-t(z_r - R)/k],$$

where R satisfies the inequalities

$$(3.13) \quad -c_1 z_r^2 \leq R \leq \frac{1}{2} s^2 z_r^2, \quad r \leq r_1.$$

If S is defined by

$$(3.14) \quad S = r^2 - z_r k^{-1} + R k^{-1},$$

formula (3.12) can be written

$$(3.15) \quad E_r^{t/k} = \exp (-r^2 t + St),$$

so that

$$(3.16) \quad E_r^{t/k} - \exp (-r^2 t) = \exp (-r^2 t) (\exp St - 1) = St \exp ((S^* - r^2)t),$$

with S^* having a value between 0 and S . The quantity S can be appraised by inserting for z_r its expression from (3.10) and by applying the inequalities (3.13) and

$$0 \leq r^2 - \sin^2 r \leq \frac{1}{6} r^4.$$

This leads to

$$(3.17) \quad -c_1 k r^4 \leq S \leq \frac{1}{24} r^4 h^2 + \frac{1}{2} s^2 k r^4$$

and therefore, if (3.2), (3.8) and (3.11) are recalled, to

$$(3.18) \quad S^* \leq S \leq \frac{1}{24} r_1^4 h^2 + \frac{1}{2} s^2 k r_1^2 r^2 \leq \frac{1}{24} p^2 + \frac{1}{4} s^2 r^2.$$

Applying the inequalities (3.17) and (3.18) to (3.16) the appraisal

$$(3.19) \quad |E_r^{t/k} - \exp (-r^2 t)| \leq t c_s (h^2 + k) r^4 \exp (-3r^2 t/4), \quad r \leq r_1$$

is obtained.

The expected improvement in the order of magnitude, when $s = \frac{1}{2}$ can be based on part c) of the Lemma in section 5, according to which

$$-c_2 z_r^3 \leq R < 0, \quad s = \frac{1}{2}$$

so that (3.17) can be replaced by

$$-c_2 k^2 r^6 \leq S \leq \frac{1}{24} r^4 h^2 \leq \frac{1}{24} p^2, \quad s = \frac{1}{2}$$

Inserted into (3.16) this leads to

$$(3.20) \quad |E_r^{t/k} - \exp(-r^2 t)| \leq t c_4 (r^4 h^2 + r^6 k^2) \exp(-r^2 t), \quad s = \frac{1}{2}, \quad r \leq r_1.$$

The quantity V_1 is now readily appraised by means of (3.3), (3.19), and (3.20). One has

$$(3.21) \quad |V_1| = \left| \sum_{r=1}^{r_1} (E_r^{t/k} - \exp(-r^2 t)) b_r \sin rx \right|$$

$$\leq t c_3 (h^2 + k) K \sum_{r=1}^{r_1} r \exp(-3r^2 t/4)$$

$$\leq t c_3 (h^2 + k) K \int_0^\infty r \exp(-3r^2 t/4) dr = c_3 K (h^2 + k),$$

and for $s = \frac{1}{2}$, in addition, in view of (3.20),

$$(3.22) \quad |V_1| \leq t c_5 K \left\{ h^2 \int_0^\infty r \exp(-r^2 t) dr + k^2 \int_0^\infty r^3 \exp(-r^2 t) dr \right\}$$

$$\leq t^{-1} c_5 K (h^2 + k^2), \quad s = \frac{1}{2}.$$

b) *The range* $r_1 < r \leq r_2$. The quantity E_r is a decreasing function of r and positive for $r < r_0$. Hence, $E_r^{t/k}$ is a positive decreasing function of r in $r < r_0$. Let r_2 be defined by

$$(3.23) \quad r_2 = [r_0]$$

(so that $r_2 = \infty$, if $r_0 = \infty$), then

$$0 \leq E_r^{t/k} \leq E_{r_1}^{t/k}, \quad r_1 \leq r \leq r_2$$

or, in view of (3.19),

$$|E_r^{t/k} - \exp(-r^2 t)| \leq E_{r_1}^{t/k} + \exp(-r_1^2 t) \leq |E_{r_1}^{t/k} - \exp(-r_1^2 t)| + \exp(-r_1^2 t)$$

$$\leq \{t c_3 (h^2 + k) r_1^4 + 1\} \exp(-r_1^2 t/2).$$

By virtue of formulas (3.3) and (3.5) this implies

$$|V_2| \leq \{t c_3 (h^2 + k) r_1^4 + 1\} \exp(-r_1^2 t/2) K \sum_{r=r_1}^{r_2} r^3.$$

The last summation is less than $\int_{r_1}^\infty r^3 dr = 2r_1^2$. Now we assume that $h_1 \leq \theta p/16$,

so that $r_1^2 > \theta p/h - 2\sqrt{\theta p/h} + 1 \geq \theta p/2h$. Then the inequality for $|V_2|$ becomes

$$(3.24) \quad |V_2| \leq \{c_7 (h^2 + k) + (8h/(\theta p)) \exp(-t\theta p/4h)\} K$$

$$\leq c_8 t^{-1} K (h^2 + k), \quad \text{for } r_1 \leq r \leq r_2.$$

c) The range $r_2 < r \leq r_3$. The set $r > r_3$ is empty, if $r_0 = \infty$. In the opposite case, E_r is a decreasing negative function in $r_0 < r < \pi/h$. Let

$$r_3 = \pi/h$$

Then, for $r_2 < r \leq r_3$,

$$\begin{aligned} |E_r^{t/k}| &= |E_r|^{t/k} = \left(\frac{4(1-s)k \sin^2(rh/2) - h^2}{4sk \sin^2(rh/2) + h^2} \right)^{t/k} \\ &\leq \left(\frac{r^2k(1-s) - 1}{r^2ks + 1} \right)^{t/k} \leq \left(\frac{r^2ks - 1}{r^2ks + 1} \right)^{t/k}. \end{aligned}$$

Here we have made use of the monotonic dependence of E_r on the variable

$$4k \sin 2rh/2.$$

As $r^2ks > r_0ks > s/(1-s)$, part b) of the Lemma in section 5 can be applied to the last bound for $|E_r^{t/k}|$, provided $s > \frac{1}{2}$. This leads to

$$(3.25) \quad |E_r^{t/k}| \leq \left(\frac{1 - 1/r^2ks}{1 + 1/r^2ks} \right)^{t/k} \leq \exp(-2t/r^2k^2s), \quad r_2 < r \leq r_3.$$

By continuity, formula (3.25) remains true for $s = \frac{1}{2}$. Hence, using (3.3) and (3.25)

$$(3.26) \quad \left| \sum_{r=r_2}^{r_3} b_r E_r^{t/k} \sin rx \right| \leq K \sum_{r=r_2}^{r_3} r^{-3} \exp(-2t/r^2k^2).$$

The function of r in the last summation assumes its maximum for $r = r_m = \sqrt{4t/3k^2}$. It is an increasing function of r for $r < r_m$, a decreasing one for $r > r_m$, and the value of the maximum is less than $t^{-3/2}k^3$. Therefore, (3.26) can be replaced by

$$\begin{aligned} (3.27) \quad \left| \sum_{r=r_2}^{r_3} b_r E_r^{t/k} \sin rx \right| &\leq K \int_0^\infty r^{-3} \exp(-2t/r^2k^2) dr + K t^{-3/2}k^3 \\ &\leq K(k^2/4t + t^{-3/2}k^3) \leq c_{10} t^{-1} K k^2, \quad \text{for } t \geq k. \end{aligned}$$

On the other hand,

$$\begin{aligned} (3.28) \quad \left| \sum_{r=r_2}^\infty b_r \exp(-r^2t) \sin rx \right| &\leq K \int_{r_2}^\infty \exp(-r^2t) r^{-3} dr \\ &= -(1/2t) \exp(-r^2t) r^{-4} \Big|_{r_2}^\infty - (2/t) \int_{r_2}^\infty \exp(-r^2t) r^{-4} dr \leq t^{-1} K r_2^{-4} \leq t^{-1} K k^2, \end{aligned}$$

because $r_2 \geq r_0 \geq ((1-s)k)^{-1}$. Combination of (3.27) and (3.28) proves that

$$(3.29) \quad |V_3| \leq c_{11} t^{-1} K k^2, \quad t \geq k.$$

d) The range $r > r_3$. For $r > r_3 = \pi/h$,

$$(3.30) \quad |V_2| \leq \sum_{r=\pi/h}^\infty |b_r| \leq K \int_{\pi/h}^\infty r^{-3} dr \leq c_{12} K h^2.$$

The desired bound for the truncation error is now obtained by adding the inequalities (3.24), (3.29), and (3.30) to (3.21) or (3.22), respectively. This completes the proof of theorem 2.

The order of magnitude of this appraisal cannot, in general, be improved. One consequence of this theorem is that the particular choice $s = \frac{1}{2}$ improves the order of magnitude of the truncation error only if $h = o(\sqrt{k})$.

As was mentioned before, it is possible to carry out the arguments of this section with the milder hypothesis

$$h^\beta/k \geq p > 0, \quad \beta > 0,$$

taking the place of (3.2). However, higher powers of t^{-1} will then appear in the bound for the truncation error. If k shrinks so much more slowly than h that

$$|\log |^{-1}/k| \leq p < \infty,$$

then the method of proof breaks down decisively.

4. Stability. The term computational stability refers to the extent to which small errors in the data and in the stepwise computation of $U(x, t)$ affect the final result. In the case of linear homogeneous difference equations the cumulative modification of the solution by such errors is the sum of the departures caused by errors on each line $t = 0, k, 2k, \dots$. Thus, a knowledge of a bound on $U(x, t)$ in terms of the initial function $f(x)$ conveys information concerning the stability of the procedure. In the previous section it was decisive that $f(x)$ had certain smoothness properties. If the round-off errors are to be treated as uniformly bounded, but otherwise arbitrary, quantities, no condition beyond (2.3) and boundedness may be imposed on $f(x)$ in the present section.

In view of the last remark it is natural to base the arguments here on the finite trigonometric interpolation series for $f(x)$, i.e., on

$$(4.1) \quad f(mh) = \sum_{r=1}^{N-1} B_r \sin mrh, \quad m = 1, 2, \dots, N-1,$$

where $N = \pi/h$ and

$$(4.2) \quad B_r = (2/N) \sum_{\rho=1}^{N-1} f(\rho h) \sin \rho rh, \quad r = 1, 2, \dots, N-1.$$

It can be directly verified that the expression

$$(4.3) \quad V(mh, nk) = \sum_{r=1}^{N-1} B_r E_r^n \sin mrh$$

solves the difference problem (1.3), (1.4) for $U(x, t)$ at the grid points $x = mh$ $t = nk, m = 1, 2, \dots, N-1; n = 1, 2, \dots$. Hence,

$$V(mh, nk) = U(mh, nk).$$

Insertion of (4.2) into (4.3) and an interchange of summations leads to

$$(4.4) \quad U(mh, nk) = \sum_{\rho=1}^{N-1} g_{\rho mn} f(\rho h)$$

with

$$(4.5) \quad g_{\rho mn} = (2/N) \sum_{r=1}^{N-1} E_r^n \sin mrh \sin prh.$$

The quantity (4.5) will now be appraised under the assumption that (2.6) and hence (2.7) is true. Moreover, the restriction

$$(4.6) \quad 0 \leq s \leq 1$$

will be imposed. Under this hypothesis E_r is a decreasing function of r , for $r \leq N-1$. Therefore, E_r^n is a decreasing function of r for all odd n , while for even n the quantity E_r^n decreases as long as $E_r \geq 0$ and increases thereafter, for $r \leq N-1$. In order to take advantage of this observation (4.5) is written in the form

$$(4.7) \quad g_{\rho mn} = (1/N) \sum_{r=0}^{N-1} E_r^n \cos(m-\rho)rh - (1/N) \sum_{r=0}^{N-1} E_r^n \cos(m+\rho)rh,$$

and each of the two right hand terms is subjected to a summation by parts. Recalling the identities

$$\sum_{r=0}^{N-1} a_r b_r = - \sum_{r=0}^{N-1} \left\{ (a_{r+1} - a_r) \sum_{\mu=0}^r b_\mu \right\} + a_N \sum_{\mu=0}^{N-1} b_\mu$$

and

$$\sum_{\mu=0}^r \cos \mu\theta = \frac{\sin(r + \frac{1}{2})\theta}{2 \sin \frac{1}{2}\theta} + \frac{1}{2} = \frac{\sin((r+1)\theta/2) \cos(r\theta/2)}{\sin \frac{1}{2}\theta}$$

one finds that

$$(4.8) \quad \left| (1/N) \sum_{r=0}^{N-1} E_r^n \cos(m-\rho)rh \right| \\ = \left| - (1/N) \sum_{r=0}^{N-1} \left\{ (E_{r+1}^n - E_r^n) \sum_{\mu=0}^r \cos(m-\rho)\mu h \right\} \right. \\ \left. + (1/N) E_N^n \sum_{\mu=0}^{N-1} \cos(m-\rho)\mu h \right| \\ \leq \frac{h}{\pi} \frac{\sum_{r=0}^{N-1} |E_r^n - E_{r+1}^n| + |E_N^n|}{\left| \sin \frac{1}{2}(m-\rho)h \right|}.$$

Now, if n is odd,

$$\sum_{r=0}^{N-1} |E_r^n - E_{r+1}^n| = \sum_{r=0}^{N-1} (E_r^n - E_{r+1}^n) = E_0^n - E_N^n \leq 2, \quad \text{odd } n.$$

If E_r is non-negative for $0 \leq r_1 \leq N$ the last formula is correct for even n as well.

But if E_r vanishes for $r = r_0$ one has, instead, with $r_2 = [r_0]$,

$$\begin{aligned} \sum_{r=0}^{N-1} |E_r^n - E_{r+1}^n| &= \sum_{r=0}^{[r_0]-1} (E_r^n - E_{r+1}^n) + |E_{r_2+1}^n - E_{r_2}^n| \\ &+ \sum_{r=r_2+1}^{N-1} (E_{r+1}^n - E_r^n) = E_0^n - E_{r_2}^n + |E_{r_2+1}^n - E_{r_2}^n| - E_{r_2+1}^n + E_N^n \leq 3, \end{aligned}$$

even n .

Inserting the result of the last two inequalities into (4.8) and taking account of the fact that both m and ρ range between 0 and $N = \pi/h$ it follows that the first right hand term in (4.7) is numerically not greater than $4 |m - \rho|^{-1}$. The second summation in (4.7) is similarly found to be bounded, numerically, by

$$4h/(\pi |\sin \frac{1}{2}(m + \rho)h|),$$

where m and ρ range from zero to π/h . For $m + \rho \leq \pi/h$ that bound is clearly not greater than $4(m + \rho)^{-1}$, which is less than $4 |m - \rho|^{-1}$. For

$$m + \rho = (2\pi/h) - \gamma, \quad 0 < \gamma < \pi/h,$$

the bound $4\gamma^{-1} = ((2\pi/h) - m - \rho)^{-1}$ is obtained, instead. But this last quantity is also not greater than $4 |m - \rho|^{-1}$, since $(2\pi/h) - m - \rho = ((\pi/h) - m) + ((\pi/h) - \rho) \geq |((\pi/h) - m) - ((\pi/h) - \rho)| = |\rho - m|$. Collecting these results it is seen that (4.7) implies the inequality

$$|g_{\rho mn}| \leq \frac{8}{|m - \rho|}.$$

On the other hand,

$$|g_{\rho mn}| \leq 2,$$

because of (2.7) and (4.5). Combination of the last two inequalities yields

$$(4.9) \quad |g_{\rho mn}| < \frac{10}{|m - \rho| + 1}.$$

Let $\bar{f}$ be defined by

$$\bar{f} = \text{l.u.b.}_{0 \leq x \leq \pi} |f(x)|.$$

Then (4.4) and (4.9) imply

$$\begin{aligned} |U(mh, nk)| &\leq 10\bar{f} \sum_{\rho=1}^{N-1} \frac{1}{|m - \rho| + 1} \\ &\leq 10\bar{f} \left\{ \int_0^m \frac{dx}{1 + m - x} + \int_m^{N-1} \frac{dx}{1 - m + x} + 1 \right\} \\ &\leq 10\bar{f}(1 + 2 \log(\pi/h)) \leq C\bar{f} \log(1/h), \end{aligned}$$

where C is a constant. This proves

THEOREM 3. *If $f(0) = f(\pi) = 0$, and $|f(x)| \leq \bar{f}$ in $0 \leq x \leq \pi$; and if*

$$2(1 - 2s)k - h^2 \leq 0, \quad 0 \leq s \leq 1,$$

then $|U(mh, nk)| \leq C\bar{f} \log 1/h$, for $0 \leq m \leq \pi/h$, $0 \leq n$. The constant C depends on h_1 only.

As a consequence of this theorem the departure caused at a grid point by the cumulative effect of all errors at grid points below that t -level is less than

$$\epsilon C\bar{f} \log (1/h)k^{-1},$$

where ϵ is an upper bound for the error committed at one point. If h_1 is small C is about equal to 10. Round-off errors of this size are considered quite manageable in numerical work.

It is an open question whether the result of theorem 3 is the best possible, i.e., if there exists a constant C^* such that corresponding to arbitrarily small values of h and k satisfying (2.6) a function $f(x)$ can be found for which

$$|U(mh, nk)| > C^*\bar{f} \log (1/h)$$

at some point $x = mh$, $t = nk$. It is well known that the factor $\log (1/h)$ can be omitted if h , k and s satisfy the inequality

$$s(1 - s)k - h^2 \leq 0,$$

for then the difference equation (1.3) satisfies a maximum principle. But this inequality is more restrictive than (2.6). For $s = \frac{1}{2}$, for instance, it implies the undesirable condition $k/h^2 \leq 1$. The boundedness statement proved in [5] is compatible with values of U of the order $O(h^{-1})$ and is therefore weaker than that of theorem 3.

5. A Lemma.

LEMMA: Let $\Phi_s(z) = \log \frac{1 - (1 - s)z}{1 + sz} + z$.

a) If $\min(sz, -(1 - s)z) \geq -\theta_1 > -1$, then

$$|\Phi_s(z)| \leq c_1 z^2, \quad c_1 \text{ a constant.}$$

b) If $0 \leq s \leq 1$, $z \geq 0$ and $(1 - s)z < 1$, then

$$\Phi_s(z) \leq \frac{1}{2}s^2 z^2.$$

c) If $z/2 \leq \theta_2 < 1$, then

$$-c_2 z^3 \leq \Phi_s(z) \leq 0, \quad c_2 \text{ a constant.}$$

Proof. a) It is readily verified that

$$(5.1) \quad \Phi_s(z) = \int_{-(1-s)z}^{sz} \frac{\tau}{1 + \tau} d\tau, \text{ if } -(1 - s)z > -1, \quad sz > -1.$$

Under the assumption of part a) one has $|1 + \tau| > 1 - \theta_1$ in the interval of integration. Hence,

$$|\Phi_s(z)| \leq (1 - \theta_1)^{-1} \int_{-(1-s)z}^{sz} |\tau| d\tau \leq c_1 z^2$$

b) Since $-(1-s)z < 0$, $sz > 0$ it follows from (5.1) that

$$\Phi_s(z) \leq \int_0^{sz} \frac{\tau}{1+\tau} d\tau \leq \int_0^{sz} \tau d\tau \leq \frac{1}{2}(sz)^2.$$

c) This result is an immediate consequence of the identity

$$\Phi_1(z) = -2 \int_0^{z/s} \frac{\tau^2}{1-\tau^2} d\tau.$$

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An Open Formula for the Numerical Integration of First Order Differential Equations (II)

By Herbert S. Wilf

In a previous paper [1], referred to below as *I*, a set of formulas was derived for the numerical integration of systems of first order differential equations. In what follows we will consider the questions of convergence and stability of the method and higher order formulas.

We quote here, for reference, the final results of *I*, namely the propagation formulas:

$$(1) \quad y_1 = y_0 + \frac{h}{12} [5f(x_0, y_0) + 8f(x_1, y_1) - f(x_2, y_2^*)]$$

$$(2) \quad y_2^* = 5y_0 - 4y_1 + 2h[f(x_0, y_0) + 2f(x_1, y_1)]$$

for the solution of

$$(3) \quad y' = f(x, y)$$

where y_0 is given.

1. Convergence. The solution of (1) and (2) for y_1 proceeds by taking as an initial guess the y_2^* from the preceding point. One then applies (2) and (1) successively until consecutive values of y_1 agree to sufficient accuracy.