

# The explicit solution of the equation of heat conduction

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In this paper we examine the  $n$ -dimensional extensions of the finite-difference schemes proposed by (a) Larkin, Lees, and Saul'yev and (b) du Fort and Frankel for the solution of the differential equation  $u_t = u_{xx}$ . The formulae obtained are explicit and stable for all values of the mesh ratios, but these ratios are found to be limited in practice by truncation error considerations. A comparison of the storage requirements and computing efficiency is made with other well known methods.

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## 1. Introduction

Consider the parabolic partial differential equation governing the conduction of heat in  $n$  space dimensions

$$u_t = \sum_{j=1}^n \frac{\partial^2 u}{\partial x_j^2}, \quad (1)$$

subject to the initial condition that  $u(x_1, x_2, \dots, x_n; 0) = f(x_1, x_2, \dots, x_n)$  where  $f$  is assumed to have a valid Fourier series expansion in the region of interest. The independent variables are taken to be bounded by  $0 \leq x_1, x_2, \dots, x_n \leq 1$  and  $t \geq 0$ , and we assume, for  $t > 0$ , that  $u$  takes the value zero on the bounding hyper-planes.

A solution to (1) is sought by embedding a grid into the region of integration and computing a finite-difference analogue of (1), at the nodal points, for as many time-steps as are deemed necessary. The following notation has been adopted:

$k$  as the step-length along the  $t$ -axis,  
 $h_j$  as the step-length along the  $x_j$ -axis,  
 $N_j = 1/h_j$ ,  $(j = 1, 2, \dots, n)$   
 $r_j = k/(h_j)^2$ .

$$\Sigma = \sum_{j=1}^n, \quad N = \prod_{j=1}^n (N_j - 1), \quad R = \sum_{j=1}^n r_j.$$

$$U = u(p_1 h_1, p_2 h_2, \dots, p_n h_n; qk) = u(p_j h_j; qk)$$

where

$$p_j = 0, 1, 2, \dots, N_j \text{ for } j = 1, 2, \dots, n.$$

Finally, we define the operators  $I$ ,  $T$ ,  $E_j$ ,  $X_j$  and  $D_j$  by

$$\begin{aligned} IU &= U, \\ T^M U &= u(p_j h_j; (q + M)k), \\ E_j^M U &= u(p_1 h_1, \dots, p_{j-1} h_{j-1}, \\ &\quad (p_j + M)h_j, p_{j+1} h_{j+1}, \dots, p_n h_n; qk), \end{aligned}$$

superfix omitted if  $M = 1$

$$X_j = E_j + E_j^{-1} - 2I,$$

$$D_j = \frac{\partial}{\partial x_j}.$$

The  $n + 1$  operators  $T$  and  $E_j$  clearly commute.

One class of methods for the solution of (1) may be written

$$(T - I)U = \sum r_j \{sT + (1 - s)I\} X_j \{U\} \quad (0 \leq s \leq 1). \quad (2)$$

The classical explicit scheme,  $(2, s = 0)$ , has its choice of the  $n$  mesh ratios  $r_j$  restricted by stability considerations, which require  $R \leq \frac{1}{2}$ .

$(2, s = 1)$  is an implicit scheme, with no stability restrictions on  $R$ , which requires the inversion of a sparse square matrix of order  $N$  at each time-step. In practice one would use  $(2, s = 1)$  only in one space dimension ( $n = 1$ ), and use the effective Alternating Direction Implicit methods of Peaceman, Rachford and Douglas [1, 8] for  $n = 2$  or 3. The A.D.I. methods avoid the necessity of inverting a widely banded matrix at each time-step and require merely the repeated cyclic inversion of  $n$  tridiagonal symmetric matrices.

We shall examine the developments of two other explicit methods for the solution of (1), namely

- the Saul'yev-Larkin-Lees semi-explicit schemes [10, 6, 7] (abbreviated to SLL schemes) which overcome the more punitive storage requirements associated with the A.D.I. methods, although at the expense of an enlarged truncation error;
- the du Fort-Frankel schemes (DUFF) which were presented for the one-dimensional case in [2], and subsequently extended by Evans [3] for the solution of  $u_{tt} + u_{xxxx} = 0$ . The  $n$ -dimensional DUFF scheme has comparable storage and computing time requirements to the analogous SLL scheme, and links between the two schemes are explored in § 5.

In § 2, we note the storage locations needed and calculations required per mesh point for the standard schemes listed below.

- Explicit  
 $(2, s = 0)$  for  $n = 1, 2, 3$ .
- Implicit  
 $(2, s = 1)$  for  $n = 1$  only.

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The A.D.I. methods of Peaceman and Rachford (PR), and Douglas and Rachford (DR) for  $n = 2$  and  $n = 3$  respectively.

In § 3 and § 4, SLL and DUFF schemes are developed, and the same computational details are noted for comparison.

## 2. Standard explicit and implicit schemes

In this, and the next two sections, we are to discuss, amongst other details, the calculations required per mesh point, and we introduce the notation  $xM + yA + zD$  to denote  $x$  multiplications and  $y$  additions/subtractions and  $z$  divisions.

### (a) Explicit

The classical explicit scheme is computed according to

$$TU = \{(1 - 2R)I + \sum r_j(E_j + E_j^{-1})\}U. \quad (3)$$

If the  $r_j$  are all unequal, the calculation of each new component of the vector  $TU$  requires  $(n + 1)M + 2nA + OD$ . However, if the  $r_j$  are all equal, each new component of the vector  $TU$  needs but  $2M + 2nA + OD$ .

It is often the case that  $R = \frac{1}{2}$ , the maximum value allowed by stability restrictions, and then the totals listed above are each reduced by  $1M + 1A + OD$  as the coefficient of  $IU$  is now zero. But more importantly, we are now able to step forward in time by computing only half the unknowns at any time-level as those unknown values of  $U$  on time-level  $q + 1$  for which  $\sum p_j$  is even(odd) are given entirely in terms of known  $U$ -values on time-level  $q$  for which  $\sum p_j$  is odd(even). It follows that we need compute over our grid only those values of  $U$  for which  $\sum p_j + q$  is either even (or odd), with a consequent halving of our expected work total.

The storage requirements can be effectively minimised to  $O(N)$  locations when  $R < \frac{1}{2}$  and  $O(N/2)$  when  $R = \frac{1}{2}$ .

### (b) Implicit

The fully explicit scheme  $(2, s = 1)$  in the space dimension may be written as

$$(I - r_1 X_1)TU = U. \quad (4)$$

In higher space dimensions,  $n = 2$  or  $3$ , we are considering not  $(2, s = 1)$  but the PR method [8] and the DR method [1], which in our notation are written

$$\left. \begin{aligned} (I - r_1 X_1)T^{1/2}U &= (I + r_2 X_2)U \\ (I - r_2 X_2)TU &= (I + r_1 X_1)T^{1/2}U \end{aligned} \right\} \text{(PR)} \quad (5)$$

and

$$\left. \begin{aligned} (I - r_1 X_1)T^{1/3}U &= (I + r_2 X_2 + r_3 X_3)U \\ (I - r_2 X_2)T^{2/3}U &= T^{1/3}U - r_2 X_2 U \\ (I - r_3 X_3)TU &= T^{2/3}U - r_3 X_3 U \end{aligned} \right\} \text{(DR)} \quad (6)$$

Thus for  $n = 1, 2$  or  $3$ , the implicit methods we are considering may be represented in the general matrix form

$$A_{jn} u_{q+j/n} = b \quad (\text{a known vector}) \quad (7)$$

for each of the  $n$  sub-steps, where the matrices  $A_{jn}$  are, under a suitable re-ordering of the grid points, block diagonal with  $N/(N_j - 1)$  leading submatrices  $C_j$  each of dimension  $N_j - 1$  ( $j = 1, 2, \dots, n$ ). Under this re-ordering, each of the  $C_j$  are of tridiagonal form, with components given by

$$(C_j)_{im} = \left. \begin{aligned} 2r_j + 1 & \quad i = m \\ -r_j & \quad i = m \pm 1 \\ 0 & \quad \text{otherwise.} \end{aligned} \right\} \quad (8)$$

As the  $A_{jn}$  are block-diagonal, each sub-block can be solved for separately, and one way of solving a matrix equation of the form (7, 8) is to split the  $C_j$  into the product factors  $L_j$  and  $U_j$  with components

$$(L_j)_{im} = \left. \begin{aligned} w_{jm} & \quad i = m \\ -r_j & \quad i = m + 1 \\ 0 & \quad \text{otherwise} \end{aligned} \right\}$$

and

$$(U_j)_{im} = \left. \begin{aligned} 1 & \quad i = m \\ t_{ji} & \quad i = m - 1 \\ 0 & \quad \text{otherwise} \end{aligned} \right\}$$

respectively, where  $L_j$  and  $U_j$  have the same dimensions as  $C_j$ . The  $\sum (2N_j - 3)$  unknowns,  $w_{jm}$  ( $m = 1, 2, \dots, N_j - 1$ ), and  $t_{ji}$  ( $i = 1, 2, \dots, N_j - 2$ ) are uniquely determined, and these decompositions are stable without interchanges due to the diagonal dominance of the  $C_j$ .

Having computed and stored the unknown elements of the matrices  $L_j$  and  $U_j$ , the number of calculations required per mesh point for each of the  $n$  substeps totals

$n = 1$	$2N + 2A + 1D$
	$r_j \text{ unequal} \quad r_j \text{ equal}$
$n = 2$	$4M + 4A + 1D \quad 3M + 4A + 1D$
$n = 3$	$5M + 6A + 1D \quad 3M + 6A + 1D$

The number of storage locations required must include registers set aside to contain the components  $w_{jm}$  and  $t_{ji}$  of  $L_j$  and  $U_j$ . For  $n = 2$ , or  $3$ , these will generally form a negligible proportion of the total. The number of locations required is then

$n = 1$	$O(3N)$
$n = 2$	$O(2N)$
$n = 3$	$O(3N)$

which are appreciable increases over the totals for the explicit schemes grouped as  $(2, s = 0)$ .

## 3. The SLL schemes

The basic SLL scheme is obtained from (2) by sharing the first term on the latter's right hand side between the forward and present time-levels. Collecting terms,

$$\{I + \sum r_j s(I - E_j)\}TU = \{I + \sum r_j(s(I - E_j) + X_j)\}U \quad (9)$$

which can be written in matrix form as

$$C(s)u_{q+1} = D(s)u_q. \quad (10)$$

$C(s)$ , the matrix representation of the space operator on the left hand side of (9), is a triangular matrix, and the solution of (10) is thus merely a process of forward substitution. (Equally well one could interchange the rôles of  $E_j$  and  $E_j^{-1}$  in (9) and produce another analogue of (1). There results a matrix problem which can be solved by backward substitution.)

Expanding (9) in the form of a Taylor series, one obtains

$$\{1 + \sum r_j s(-h_j D_j - h_j^2 D_j^2/2 - h_j^3 D_j^3/6 - \dots)\} \\ ku_t + k^2 u_{tt}/2 + \dots = 2\sum r_j (h_j^2 D_j^2/2 + h_j^4 D_j^4/24 + \dots) u,$$

i.e.

$$u_t = \sum (D_j^2 u + h_j^2 D_j^4/12 + sk/h_j D_j u_t + sk^2/h_j D_j u_{tt}) \\ + \frac{k}{2} (s D_j^2 u_t - u_{tt}) + \dots \\ = \sum D_j^2 u + O(h^2 + (1-s)k + k/h).$$

Thus as  $h_j \rightarrow 0$  and  $k \rightarrow 0$ , we also require  $k/h_j \rightarrow 0$  ( $j = 1, 2, \dots, n$ ) for the scheme (9) to converge to the correct differential equation (1) (unless  $s = 0$ , in which case the scheme is the classical explicit formula (2,  $s = 0$ )). If the step lengths are equal and we take

$$h_j = h, r_j = r \quad (j = 1, 2, \dots, n),$$

then in practice this implies that  $k/h = hr$  be 'small', which is more favourable as  $h$  decreases. The results of some numerical experiments are presented in § 6, and further comments on this scheme are left until there.

As the matrix  $C(s)^{-1}D(s)$  does not have known eigenvalues, we analyse the stability of (16) by the Fourier series method. This assumes a set of errors  $e(p_j h_j; q)$  exists at the grid point  $(p_1 h_1, p_2 h_2, \dots, p_n h_n; qk)$ , and that  $e(p_j h_j; q)$  has the finite trigonometric expansion

$$e(p_j h_j; q) = \sum_{t_1=1}^{N_1-1} \dots \sum_{t_n=1}^{N_n-1} A(p_j; q) \prod_{m=1}^n \exp(ic_m p_m)$$

where  $c_m = \pi t_m h_m$ , and  $A(p_j; q)$  represents the Fourier coefficients which are not required. Stability is assured if

$$|1 + \sum r_j s(1 - \exp(ic_m))| \geq |1 + \sum r_j s(1 - \exp(ic_m)) \\ + 2 \sum r_j (\cos(c_m) - 1)|$$

which implies

$$1 + s \sum r_j (1 - \cos(c_m)) \geq \sum r_j (1 - \cos(c_m))$$

i.e.

$$R \leq \frac{1}{2(1-s)}.$$

That  $R$  is not restricted when  $s = 1$  agrees with results given by Larkin [6]. In the one dimensional case, this bound is certainly better than that derived by analysis of the spectral norm of the matrix  $C(s)^{-1}D(s)$  (see [10], p. 37), and is considerably easier to obtain. In higher

space dimensions, the work involved in attempting to obtain the stability criterion by spectral analysis would seem to be formidable.

Both Saul'yev [10] and Larkin [6] suggested ways of improving (9). As (9) is unconditionally stable only for  $s = 1$ , we follow Larkin in only using that value of  $s$  for the suggested improvements. In this case, (9) simplifies into

$$(T - I)U = \sum r_j \{(E_j - I)T + (E_j^{-1} - I)\}U, \quad (11)$$

and another scheme with similar properties is

$$(T - I)U = \sum r_j \{(E_j^{-1} - I)T + (E_j - I)\}U. \quad (12)$$

(i) Saul'yev and Larkin suggested using these alternately to produce an estimate of  $T^2 U$  from  $U$  via  $TU$  by the formulae

$$\{I + \sum r_j (I - E_j)\}TU = \{I - \sum r_j (I - E_j^{-1})\}U \\ \{I + \sum r_j (I - E_j^{-1})\}T^2 U = \{I - \sum r_j (I - E_j)\}TU. \quad (13)$$

Elimination of  $TU$  yields

$$\{I - \sum r_j X_j + \sum r_j (I - E_j^{-1}) \sum r_j (I - E_j)\}T^2 U \\ = \{I + \sum r_j X_j + \sum r_j (I - E_j^{-1}) \sum r_j (I - E_j)\}U.$$

Whilst this alternating scheme is obviously unconditionally stable, examination of the truncation error, assuming a valid Taylor expansion, shows (13) to approximate the equation

$$u_t = \sum (D_j^2 u + h_j^2 D_j^4 u/12) + (\sum (k/h_j)^2 D_j^2 u_t) \\ - k(u_{tt} - \sum D_j^2 u_t) + \dots$$

which represents (1) to within a truncation error of  $O(h^2 + k^2 + (k/h)^2)$ . This is a useful improvement for small  $(k/h)$ , and the scheme (13) requires neither extra storage nor computing time over (11) or (12) alone.

(ii) Saul'yev and Larkin also proposed using (11) and (12) together to produce an averaged scheme for the solution of (1). It follows that such a scheme is equivalent to

$$\{I + \sum r_j (I - E_j)\}\{I + \sum r_j (I - E_j^{-1})\}TU \\ = \frac{1}{2}\{2 - [\sum r_j (I - E_j)]^2 - [\sum r_j (I - E_j^{-1})]^2\}U. \quad (14)$$

Saul'yev suggested treating (14) as a new formula and solving it in that form, Larkin in the more tractable form of solving for  $TU$  by both (11) and (12) separately, and then averaging. The truncation error of this scheme, which has the same left hand side operator as (13), clearly contains a term of  $O(k^2/h^2)$ .

It requires double the computing time and storage space of (11, 12, 13) but it would be the only SLL scheme to give symmetric solutions to symmetric problems.

In  $n$  space dimensions, both the basic SLL schemes (11, 12) and the alternating form (13) require  $(n+1)M + 2nA + OD$  calculations per point when the  $r_j$  are unequal, and  $2M + 2nA + OD$  if the  $r_j$  are all equal. If  $R = 1$ , both these totals are reduced by  $1M + 1A + OD$ . However, there is no possibility with these schemes of computing over alternate points, as with the classical explicit scheme (2,  $s = 0$ ), and so the work total for

(11, 12, 13) with  $R = 1$  is the same as for (2,  $s = 0$ ) with  $R = \frac{1}{2}$ . The number of storage locations required is  $O(N)$ .

For the Larkin averaged scheme (29), these totals are doubled.

#### 4. Truncation error and stability of the DUFF schemes

Du Fort and Frankel [2] suggested (for  $n = 1$  only) taking the unstable three-level Richardson scheme and amending it by sharing the coefficient of  $U$  in it equally between  $TU$  and  $T^{-1}U$ .

In  $n$  dimensions, we would approximate (1) by

$$(T - T^{-1})U = 2\Sigma r_j(E_j + E_j^{-1} - T - T^{-1})U. \quad (15)$$

A Taylor series expansion yields

$$2ku_t + k^3u_{ttt}/3 + \dots = 2\Sigma\{kD_j^2u + kh_j^2D_j^4u/12 + \dots - (k^3/h_j^2)u_{tt} - (k^5/h_j^2)u_{tttt}/12 - \dots$$

or

$$u_t = \Sigma(D_j^2u + h_j^2D_j^4u/12 - (k/h_j)^2u_{tt}) - k^2u_{ttt}/6 + \dots$$

i.e.

$$u_t = \Sigma D_j^2u + O(h^2 + k^2 + n(k/h)^2).$$

For the stability analysis, we use the method detailed in Householder [5]. We write the finite difference analogue in matrix form as

$$(1 + 2R)u_{n+1} = 2\Sigma r_j Y_j u_n + (1 - 2R)u_{n-1}$$

where the  $n$  matrices  $Y_j$  are each representations of the operators  $E_j + E_j^{-1}$ . The  $Y_j$  thus have known eigenvalues and common eigenvectors. It follows from Householder's analysis that the stability of (15) hinges on the magnitudes of the roots of the quadratic equation

$$(1 + 2R)\mu^2 - 2\Sigma r_j y_j \mu - (1 - 2R) = 0. \quad (16)$$

We have stability if  $|\mu_i| \leq 1$  whenever the  $y_j$  are replaced by eigenvalues of the corresponding  $Y_j$ . Since the  $y_j$  are of the form  $y_j = 2 \cos(\pi p_j h_j)$ , it follows that  $|\Sigma r_j y_j| < 2R$  and accordingly there is a  $v$ , dependent upon  $y_j$ , such that (16) may be replaced by

$$(1 + 2R)\mu^2 - 4R \cos v \cdot \mu - (1 - 2R) = 0 \quad (17)$$

for any choice of  $y_j$ .

If the roots of (17) are complex, then they have equal modulus and

$$|\mu|^2 = |(1 - 2R)/(1 + 2R)| < 1.$$

If the roots of (17) are real, then

$$\mu = \frac{2R \cos v \pm \sqrt{[4R^2 \cos^2 v + (1 - 4R^2)]}}{(1 + 2R)}$$

and since  $R > 0$  and  $0 < v < \pi$ , this implies

$$0 < 4R^2 \cos^2 v + 1 - 4R^2 < 1,$$

and it follows that  $|\mu_i| < 1$ .

We note that if  $1 - 2R = 0$ , then (15) becomes a two level scheme and then that one of the roots of (17) is zero. In this case, DUFF scheme (15) becomes identical to (7,  $s = 0$ ) when  $R = \frac{1}{2}$  in both formulae.

In [2], du Fort and Frankel pointed out that the computations using (15,  $n = 1$ ) could be performed in two ways—under their so called 'leap frog' and 'pyramid' orderings. Both of these are of interest and both extend easily to  $n > 1$ .

In the leap frog ordering only one-half of the mesh values need be computed. For consider (15) for the calculation of the approximation to  $u(p_j h_j; (p + 1)k)$ . Let us denote all points for which  $q + \Sigma p_j$  is even as E points, and odd as O points. Then all mesh points considered are either E or O points and from (15) it follows that if  $(p_j h_j; (q + 1)k)$  is an E(O) then it is computed entirely in terms of E(O) points so that in the course of using (15), only E or only O points need be computed and stored. Thus as the computations proceed from time-level to time-level, we calculate successively the points for which  $\Sigma p_j$  is even on one time-level and odd on the next, or vice versa.

Under the pyramid ordering we compute over one of the planes  $t \pm \Sigma p_j h_j = \text{constant}$ . Taking the positive sign, this reduces to a two level scheme centred on  $(p_j h_j; t')$ , where  $t' = t + \Sigma x_j$ , and yet omitting that time-level. In full

$$(T - T^{-1})U = 2\Sigma r_j \{(E_j - I)T + (E_j^{-1} - I)T^{-1}\}U \quad (18)$$

which can be used over planes  $t'$  even, or  $t'$  odd, without reference to intermediate levels.

Both these orderings reduce the expected work totals and locations required by one-half. Per point we perform  $(n + 1)M + 2nA + OD$  calculations for  $r_j$  unequal and  $2M + 2nA + OD$  for  $r_j$  all equal. If  $R = \frac{1}{2}$ , the leap frog scheme becomes two level, and the totals listed above are each reduced by  $1M + 1A + OD$ .  $O(N)$  locations are needed for general  $R$  under both orderings.

#### 5. Links between SLL and DUFF schemes

We first note that the DUFF leap frog and pyramid schemes are centred about a mid time level, whereas the SLL schemes are expanded about the backward level. Suppose now we do an SLL-type expansion on the classical unstable Richardson scheme instead of (2), sharing the right hand side of (1) between the forward and backward time-levels in the manner of (11, 12). This yields a formula identical to (18) in form, but one which is computed over lines  $t = \text{constant}$ . It is easy to show that with this ordering the formula is stable for all values of  $r_j$  and has truncation error of  $O(h^2 + k^2 + k/h)$ . It can, of course, be used in an alternating manner which further improves this to  $O(h^2 + k^2 + k^2/h^2)$ .† Since this new scheme can be computed over alternate time-levels then it requires no

† In § 6, these schemes are denoted by SLL\*.

more storage space than (9,  $s = 1$ ). We have thus shown that this new SLL-type scheme and the DUFF pyramid scheme correspond exactly when computed over the points  $(p_j h_j; t)$  and  $(p_j h_j; t + \Sigma p_j h_j)$  respectively.

Now, consider the solution of the elliptic equation

$$\Sigma D_j^2 u = b(p_j h_j) \quad (19)$$

(in matrix form

$$(I - L - U)x = b)$$

by (a) successive over-relaxation; (b) fixed parameter first and second order Richardson methods.

(a) It is easy to show that the equation governing the error  $e^n$  of the  $n$ th iteration in the solution of (19) by S.O.R. is

$$e^{n+1} - e^n = \omega \Sigma (E_j e^{n+1} + E_j^{-1} e^n - 2Ie^n) / (2zh_j^2),$$

where  $z = \Sigma 1/h_j^2$  and  $\omega$  is the successive over-relaxation parameter. This may be rewritten as

$$e^{n+1} - e^n = (\omega/z(2 - \omega)) \cdot \Sigma \{ (E_j - I)e^{n+1} + (E_j^{-1} - I)e^n / h_j^2 \} \quad (20)$$

i.e. the altering of  $2Ie^n$  into  $2Ie^{n+1}$  has no effect on convergence provided that  $\omega$  is altered as shown. Now (20) is the same form as DUFF pyramid and the new SLL scheme, with

$$\omega/(z(2 - \omega)) = 2k \quad \text{or} \quad \omega = 4R/(1 + 2R).$$

Thus  $0 < \omega < 2$ , and this completes the correspondence.

(b) The solution of (19) by the first-order, single parameter ( $\alpha$ ) Richardson scheme yields an error equation

$$e^{n+1} - e^n = (\alpha/2z) \cdot \Sigma X_j e^n / h_j^2$$

which is of the same form as (7,  $s = 0$ ) with

$$\alpha/2z = k \quad \text{i.e.} \quad R = 2\alpha.$$

Using the second-order Richardson method with fixed parameters,  $\alpha$  and  $\beta$ , the error in the solution of (19) obeys the equation

$$e^{n+1} - e^n = (\alpha/2z) \cdot \Sigma X_j e^n / h_j^2 + \beta(e^n - e^{n-1})$$

which corresponds to DUFF leap frog with

$\alpha/2z = 2k/(1 + 2kz)$  and  $\beta = (2kz - 1)/(2kz + 1)$ . If  $\alpha$  and  $\beta$  take their optimum values

$$\alpha = 4/(\sqrt{a} + \sqrt{b})^2 \quad \text{and} \quad \beta = \frac{(\sqrt{a} - \sqrt{b})^2}{(\sqrt{a} + \sqrt{b})^2},$$

where  $a$  and  $b$  are the maximum and minimum eigenvalues of  $I - L - U$ , then  $a, b = -1 \pm \sqrt{1 - 1/R^2}$ .

## 6. Numerical results and comments

The methods outlined were programmed to solve parabolic problems in one, two and three space dimensions. One such problem was

$$u_t = u_{xx} : u(0, t) = u(1, t) = 0, \quad t \geq 0$$

subject to the initial condition

$$f_1(x) = u(x, 0) = \sin(\pi x).$$

For various values of  $h$  and  $r$ , computed results for  $10^5 \cdot u(0.5, t)$  are listed in Table 1 in the format group

$$u(0.5, 0.2)$$

$$u(0.5, 0.4).$$

The rounded analytic solutions for  $10^5 u$  are

$$13891$$

$$1930.$$

Further numerical problems included the initial values

$$f_2(x) = \begin{matrix} 1 & 0 < x < 1 \\ 0 & x = 0, 1 \end{matrix}$$

and

$$f_3(x) = 1 - |1 - 2x|,$$

and analogues of all three in higher space dimensions. The results quoted in Table 1 give an indication of the behaviour in the remaining problems.

Typically, we note that with the SLL and DUFF schemes the error does indeed diminish with decreasing  $k/h$ , and also that the Averaged SLL (14) and Alternating SLL (13) schemes give very similar results.

In this example, the basic SLL scheme (9) gives better results than either (13) or (14). This is not always so—a counter-example is provided by the methods of Evans [3] and Fairweather and Gourlay [4] for the solution of  $u_{tt} + u_{xxxx} = 0$ . Their solutions are achieved by splitting the fourth-order equation into an equivalent, simultaneous second-order pair  $v_t = w_{xx}$ ,  $w_t = -v_{xx}$ , each of which can then be solved by our techniques. Given

$$v(x, 0) = x - x^2 \quad 0 \leq x \leq 1$$

$$w(x, 0) = 0$$

$$v(0, t) = v(1, t) = w(0, t) = w(1, t) = 0,$$

Table 2 lists the error in computed values of  $u$  for  $x = 0.1, 0.2, \dots, 0.5$  at  $t = 0.02$  for  $h = 0.05$  and  $r = \frac{1}{2}$  for SLL (9) and the Alternating SLL (13) schemes.

Table 2

Error in  $10^7 \cdot u$

VALUE OF  $x$

METHOD	0.1	0.2	0.3	0.4	0.5
SLL	-301	-619	-669	-510	-134
AV.SLL	12	63	43	-7	-47

Error in  $10^6 \cdot u_{xx}$

SLL	331	2726	1694	2503	2555
AV.SLL	301	924	442	202	290

Table 1

Value of  $10^5 \cdot u$ 

$r = 1/2$					$r = 2$				
VALUE OF $h$					VALUE OF $h$				
METHOD	$h=1/10$	$h=1/20$	$h=1/40$	$h=1/80$	METHOD	$h=1/10$	$h=1/20$	$h=1/40$	$h=1/80$
IMPLICIT	13435 1805	13778 1898	13863 1922	13884	SLL	12871 1434	13661 1811	13835 1900	13877
SLL	14047 1960	13930 1937	13901 1931	13894	ALT.SLL	22754 5191	16401 2686	14551 2117	14060
ALT.SLL	14658 2146	14101 1988	13946 1945	13905	AV.SLL	20143 4000	16068 2572	14511 2104	14055
AV.SLL	14599 2129	14094 1986	13945 1945	13905	DUFF	634 -635	11127 1216	13223 1747	13725
DUFF	13435 1805	13779 1898	13863 1922	13884	SLL*	8361 -892	12710 1389	13620 1799	13825
SLL*	13829 1858	13877 1912	13888 1925	13890	ALT.SLL*		23538 5548	16485 2716	14556
ALT.SLL*	16292 2647	14560 2119	14067 1979	13936					
$r = 1$					$r = 4$				
VALUE OF $h$					VALUE OF $h$				
METHOD	$h=1/10$	$h=1/20$	$h=1/40$	$h=1/80$	METHOD	$h=1/10$	$h=1/20$	$h=1/40$	$h=1/80$
SLL	13829 1858	13877 1912	13888 1925	13890	SLL	8361 -892	12710 1389	13620 1799	13825
ALT.SLL	16292 2647	14560 2119	14067 1979	13936	ALT.SLL	18704 3712	23538 5548	16485 2716	14556
AV.SLL	15877 2508	14511 2104	14061 1977	13935	AV.SLL	31716 10010	21566 4600	16230 2627	14525
DUFF	11354 1265	13268 1759	13736 1887	13852	DUFF	-29408 -32425	-35 -654	11061 1203	13211
SLL*	12871 1434	13661 1811	13835 1900	13877	SLL*		8276 -953	12670 1378	13609
ALT.SLL*	22754 5191	16401 2686	14551 2117	14060	ALT.SLL*		44392 20254	23918 5725	16533

In computing the SLL solutions in the one dimensional case, we are in fact solving a scheme representing

$$\alpha u_{xt} + u_t = u_{xx}$$

for 'small'  $\alpha$ . Subjected to the transformation

$$x \rightarrow x$$

$$t \rightarrow t + \alpha x/2$$

this equation becomes

$$\frac{\alpha^2}{4} u_{tt} + u_t = u_{xx} \quad (21)$$

(which is also the form of the DUFF scheme in one space dimension). It is easy to show that if the attenuation factor to  $u_t = u_{xx}$  is  $\lambda$ , say, then the corresponding attenuation factors to (21) are

$$2\{-1 \pm \sqrt{(1 + \lambda\alpha^2)}\}/\alpha^2$$

or

$$-\frac{4}{\alpha^2} + \dots$$

~

$$\lambda - \frac{1}{4} \alpha^2 \lambda^2 + \dots$$

This shows why  $\alpha$  'small' is a necessary condition for an accurate solution. (See also du Fort and Frankel [2], pp. 142–144.)

The reported results seem to indicate that out of the range of SLL and DUFF schemes (9) and (13) are to be preferred, and that a 'small value' of  $(h/k)$  would be less than  $1/40$ , say. For very small values of  $h$  ( $1/80$  or less) the schemes (9) and (13) can still therefore be competitive.

From the list of operations necessary per point, it can be seen that the Implicit and A.D.I. methods are not much more expensive than the Explicit schemes, and one

can use a large value of  $R$  in them with more safety than in SLL schemes. Although they do require more working space, this is only likely to be serious in three dimensional problems on a small computer.

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## Book Review

*Numerical Integration*, by P. J. DAVIS and P. RABINOWITZ, 1967; 230 pp. (Waltham, Massachusetts: Blaisdell Publishing Company, \$7.50.)

This monograph is intended to give a concise but comprehensive account of the available formulas and methods for the numerical evaluation of integrals. The subject is presented from the application point of view and the treatment is modern and computer oriented.

Chapter 1 contains an introduction to the concept of numerical integration and also gives some useful analytical background material. Chapter 2, by far the longest, deals with approximate integration over a finite interval and includes special sections on the treatment of periodic functions, rapidly oscillatory functions, contour integrals, improper integrals and indefinite integration. In Chapter 3 is a brief description of special methods and formulas for integration over an infinite range, while Chapter 4 covers the subject of error analysis and includes a treatment of the effect of round-off error following the general analysis given by J. H. Wilkinson. The effect of truncation error is analysed through Peano's theorem, differences, the theory of analytic functions,

and functional analysis. The topic of multi-dimensional integrals follows and includes a large section devoted to Monte Carlo methods. The last chapter deals with automatic integration schemes, which are classified as adaptive or non-adaptive and iterative or non-iterative, and has special sections devoted to Romberg's scheme and methods using Chebyshev polynomials. The book is concluded by five appendices containing a reprint of the article 'On the Practical Evaluation of Integrals' by M. Abramowitz, some FORTRAN programs, and bibliographies of ALGOL procedures, tables, books and articles.

The text is exceptionally well written, and very well organised, and the link between theory and application is, throughout, strongly forged with the help of numerous illustrative examples. The authors have carefully dug into the literature and concluded each section with a useful set of references. The book is a 'must' for any one interested in the practical evaluation of integrals, and will undoubtedly be of great value to all who wish to make a serious study of numerical integration.

P. C. CHAKRAVARTI (London)