ON THE SOLUTION OF PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS BY DIFFERENCE METHODS

by

A.S. Douglas

Director, Computation Laboratories,
University of Leeds

1. INTRODUCTION

Parabolic partial differential equations are important in physics, chemistry and biology. There are a number of interesting problems involving diffusion of heat, of particles or of elementary organisms through solids, gases or liquids. These give rise to diffusion equations, the simplest form of which can be written

$$\nabla^2 \phi = \partial \phi / \partial t \qquad (1),$$

where the value of ϕ is given over the space boundaries for all t, and an initial distribution of which over all space is known.[1.] It is usually required to solve for ϕ at successive steps in t. For simplicity we shall confine our remarks to the case of a single space variable for the present, although some of the results are more general than this.

It can be shown[2.] that certain elliptic equations involving eigenvalues can also be solved by recourse to solution of a related parabolic equation. Let us consider the equation

$$d^2P/dr^2 + 2 \left\{ E - V(r) \right\} P = 0 \qquad (2),$$

where $P(0) = P(\infty) = 0$. Solutions of this exist for a set of eigenvalues, E_n, of E, which are all negative. We order these such that $E_0 < E_1 < E_2$ etc. Let the corresponding eigen-functions be $P_n(r)$; these may be supposed to form a complete set. We consider now the equation

$$\partial^2 Y / \partial r^2 + 2 \left\{ E^* - V(r) \right\} Y = \partial Y / \partial t \qquad (3),$$

where $Y(0) = Y(\infty) = 0$ for all t. We may write $Y = \sum_n a_n(t) P_n(r)$, since the P_n form a complete set. Substituting in equation (3) we find that $a_n(t) = \exp 2(E^* - E_n)t$. If we choose E^* such that $E_0 < E^* < E_1$, then only a_0 is an increasing function of t. We deduce that $Y \rightarrow P_0 \exp 2(E^* - E_0)t$ as t increases. We may eliminate the exponential by dividing through the solution of Y at each step in t by the value of $Y(r_s)$, where r_s is any value of r in the range $(0, \infty)$. Thus $Y(r)/Y(r_s) \rightarrow P_0(r)/P_0(r_s)$, as $t \rightarrow \infty$.

This result can readily be generalised to many space variables.

If we replace equation (3) by its 'forward difference' equivalent, we derive the equation

$$s\left\{ y(r_{j+1},t) - 2y(r_j,t) + y(r_{j-1},t) \right\} + 2\delta t \left\{ E^* - V(r_j) \right\} y(r_j,t)$$

$$= y(r_j,\ t + \delta t) - y(r_j,t) \qquad (4),$$

where $s = \delta t / \delta r^2$, $j = 1,2,\ldots\ n-1$, $r_0 = 0$, $y(r_0) = 0$ and r_n is sufficiently large that $y(r_n)$ is negligible. For $s = \frac{1}{2}$, this is exactly the equation derived from stochastic considerations by King,[3] and solved by him using a 'random walk' process to give solutions for the ground state wave function of the Simple Harmonic Oscillator[4]. The equation can, of course, be solved also by direct iteration, and this has been carried out successfully by the author[5], both for the Simple Harmonic Oscillator and also for the ground state solution of the Hydrogen equation. An accuracy of better than 1% was achieved for the latter function after about 200 iterations (with suitable choice of δr). The solution took about 40 minutes using EDSAC I.

It is apparent that the solution of some elliptic equations can be carried out by a pseudo-diffusion process, the auxiliary variable t being introduced artificially to set up an iteration procedure. It is, perhaps, not generally realised that the normal n-step or iterative processes of solution of an elliptic equation, such as relaxation or even matrix methods, effectively introduce such an auxiliary variable in order to achieve their object. The solution of elliptic equations by such a method has been recently discussed by Young.[6]

The essential difference between the solution of elliptic equations by use of a related parabolic equation, and solution of a diffusion equation is in the result which is required to be achieved. In the latter case we are interested in the values of the function at all intermediate values of t, but usually only qualitatively in the asymptotic behaviour. In the former case we are interested exclusively in the asymptotic behaviour for large t. The numerical analytical approach, therefore, differs markedly in each case. We shall refer to them as Case I and Case II respectively.

In either case, of course, we are interested in showing that solutions of the differential equations exist. In practical cases such existence is usually assured. If difference methods are to be used, our next concern is to decide what difference replacement is to be used for the differential equation. For Case I we require that the divergence of the solution to the difference equation from the solution of the differential equation should be small and calculable in terms of known quantities after a finite number of steps in t - the fewer the better. For Case II we require that the divergence should be as small as possible at each of a prescribed set of steps in t. In each case the steps in r are governed by the accuracy to which it is required to represent the function, and may be regarded as fixed for a given problem.

2. THE DIFFERENCE REPLACEMENT

In order to ensure that any divergence between the solution of the difference equation and the required solution of the differential equation remains small and calculable it is desirable to exclude any solutions of the difference system which do not correspond to solutions of the differential equation. Thus, since the differential equation is second order in the space variables and first order in t, the difference equation should be of the same order in those variables. For a single space variable at most three points in r at two different values of t should be used. This, nevertheless, permits some latitude in the choice of difference replacements. The general replacement has been considered by Collatz [7], and a form symmetric in r has been investigated by Crandall [8]. We may write this in the form:

$$s\left\{(1-a)\delta_0^{\,2} + a\delta_1^{\,2}\right\} w = \Delta_0 w \qquad (5),$$

where $s = \delta t/\delta r^2$, $\delta_m^{\,2} w = w(r_{j+1},t_m) - 2w(r_j,t_m) + w(r_{j-1},t_m)$ $\Delta_k w$

$= w(r_j,t_{k+1}) - w(r_j,t_k)$, and a is an arbitrary constant less than unity.

The cases a = 0, 1 have been discussed by O'Brien, Hyman & Kaplan, and it has been shown that, for a = 0, $s < \frac{1}{2}$ [9]. Crank and Nicholson [10] applied the value $a = \frac{1}{2}$ and have shown that, in this case, there is no restriction on the choice of s imposed by considerations of cumulative rounding error, or 'stability'. The convergence of both the process for a = 0 for $a = \frac{1}{2}$ to the solution of the differential equation has been proved under fairly wide conditions by Juncosa & Young [11] and the order of convergence established. For a = 0, Milne [12] gives the result that the increase in error at each step in t is $O(h^6)$ if s is chosen as $1/6$. These results have been extended by Crandall (for s of order 1) from equation (5). He shows that the largest value of s for which the increase in error is $O(h^6)$ at each step in t is determined by the intersection of the two curves, $a = \frac{1}{2}(1-1/6s)$ and $a = \frac{1}{2}(1-\frac{1}{2}s)$, giving the result $a = (3-\sqrt{5})/6$, $s = \sqrt{5}/10$.

Whilst this choice is satisfactory for Case II applications, it is less satisfactory for Case I, since we are then concerned with rapid approach to an asymptotic behaviour, and accuracy at intermediate steps of the calculation is not important. We are free to use the Crank & Nicholson procedure, or indeed any procedure for which $a > \frac{1}{2}$, with any value of s, and some suitable choice of a such as this is attractive. However, in using an electronic computer the obvious advantages of using a large step in t must be weighed against the additional complication in procedure at each step in t introduced by any 'implicit' process. Whereas for a = 0 we may evaluate $w(r_j,t_{k+1})$ from set of w at t_k, an implicit procedure involves the inversion of a matrix initially and multiplication of the $w(r_j,t_k)$, regarded as a vector in r, by that matrix for each successive step in t. It is our experience that the use of the Crank-Nicholson process is to be preferred to the forward difference procedure, since s may often be chosen as large as 4, and the vector multiplication is not eight times the work at each step in t.

Processes based on equation (5) are not the only possible methods of solution of the general difference equation. An alternative stable system has been investigated by Frankel & DuFort[13]. This utilises a difference replacement using only the allowed set of points in r and t, but is not symmetric in r. In order to achieve stability and convergence to the required answer the process is not applied to successive points in r, but to alternate points on one traverse of the range, followed by application to the intermediate points on the second traverse. The two superposed grids are, of course, linked at each step. The process uses larger steps in t, but is a little more complicated to compute at each point than the forward difference procedure. It still suffers by comparison with 'implicit' procedures based on equation (5), however.

3. RICHARDSON'S PURIFICATION PROCESS

All the procedures described above are based on the parameter s remaining constant over all t. Richardson[14] considered the difference replacement as creating a procedure by which $w(r_j,t_{k+1})$ is derived from $w(r_j, t_k)$ by adding the result of a linear operation on the w at t_k. Writing $w(r_j,t_{k+1}) = w(r_j,t_k) + Lw(r,t_k)$, we note that the linear operator L must possess a set of eigenvalues. Richardson pointed out that, writing $L = s\delta^2 w$ say, the choice of s near an eigenvalue, s_i, would reduce the component due to that eigenvalue in the difference between the values of w at t_{k+1} and t_k. Consequently, for a Case I application it is desirable to choose s near the principal s_i affecting the difference between the w at t_k and the asymptotic value of w. Since we do not know which s_k is most important, Richardson proposed the use of different values of s as k increased, the particular s_k being chosen on the basis of experience. This approach has been applied recently by Leigh[15], and he has shown that the restrictions on s derived from equation (5) may be broken occasionally without instability resulting.

It has been shown by Peaceman & Rachford[16] that from equation (5), we may deduce a set of eigenvalues for the s, but they have not linked this with Richardson's procedure. If we write $\Delta_{k+1} w = B\Delta_k w$, where B is a parameter independent of r, we may derive from equation (5) the equation

$$\Delta_0 w(r_{j+1}) + \Delta_0 w(r_{j-1}) + (-2+p)\ \Delta_0 w(r_j) = 0 \qquad (6),$$

where $p = (1-B)/s(1-a+aB)$. Since $\Delta_0 w(r_0) = \Delta_0 w(r_n) = 0$, we may show that p possesses a set of eigenvalues, p_i, given by $p_i = 4\sin^2(i\pi/2N)$, $i = 1,2....N-1$, where N is the number of points of tabulation over the range $(r_0 r_n)$. Corresponding to each eigenvalue is an eigenvector $\Delta_0 w_i(r_j)$, called a 'normal mode' of the system. If no mode is to oscillate, then we require $B \leq$. It is from this condition that the restrictions on s given above are derived. Now let us suppose we choose $B = 0$, and treat s as a parameter with eigenvalues. Clearly none of the corresponding modes will oscillate, and we ought to achieve the maximum rate of convergence by using the resulting eigenvalues in Richardson's process.

Before we can apply this, however, we must amend the analysis to take account of s being changed from step to step. Equation (6) still holds, but we now have $p = (1/s_0 - B/s_1)/(1 - a+aB)$. The stability analysis is no longer straightforward, but we may deduce that, if $a \geq \frac{1}{2}$, and s_0 and s_1 are each greater than $\frac{1}{4}$, then $B < 1$ if $(1/s_0 - 1/s_1) < 4 \sin^2 (\pi/2N)$. Extrapolating N to infinity this implies s_1 must be less than s_0, but in practice this rule need not be observed very closely. In particular, if we choose for s at t_k the successive eigenvalues, s_k, given by taking $B = 0$ and $p_k = 4 \sin^2 (k\pi/2N)$, then the requisite conditions are fulfilled for stability, provided we take $a \geq \frac{1}{2}$.

If we use the exact values for the s_k, then Richardson's process is no longer strictly iterative, but becomes an N-step procedure. However, it is not usually possible to use the largest eigenvalues, since δt is then so large that the error terms dependent upon it become significant. Nevertheless, the procedure has been successfully applied to a modified form of the diffusion equation described below. Compared with the normal Crank-Nicholson process, convergence is considerably more rapid, but it is necessary to invert a matrix at each step in t, thus involving at least double the amount of work. In spite of this, results were encouraging and the total time taken to obtain similar standards of accuracy by the two methods favoured the modified Richardson procedure.

4. THE MODIFIED DIFFUSION EQUATION

It was pointed out in the introduction that it is possible to obtain solution of equations of the form of equation (2) by solution of the related equation (3). In carrying out difference replacement of the derivatives of such an equation the relevant considerations have been discussed above. Replacement of the extra term, however, must be considered, and a general approach is to replace Y by $(1-b)\, w(r_j,t_k) + b w(r_j,t_{k+1})$, where b is a constant less than unity. A stability analysis along the lines of that given in the previous section leads to equation (6) with $p = \left\{ \left[1+2s_0\delta r^2 \quad (1-b)\left\{ E^*-V(r_j) \right\} \right] /s_0 - B \left\{ 1-2s_1\delta r^2 b \left[E^*- V(r_j) \right] \right\} /s_1 \right\} /(1-a+aB)$. If we choose $B = 0$, $b = 1$, then p has the same value as if the extra term were not included, and so we may ignore its effect upon the solution.

The equation for the ground state wave function of the Simple Harmonic Oscillator has been solved by Phelps[17]. using the replacement $a = \frac{1}{2}$, $b = 1$. Comparisons were made between the accuracy achieved over various parts of the range after a fixed number of steps in t for this process and for the process using a fixed value of s. In each case the same r was used, and it was chosen sufficiently small that the term containing E was not significantly large for values of s around $s = 1$. About 50 steps in r were taken across the range (0,00). Roughly speaking the Richardson process gave high accuracy after less than 30 steps in t, whilst a comparable accuracy was achieved for $s = 2$ after about 100 steps in t. It is to be noted that the eigenvalues were used in ascending order, and the larger ones omitted. No significant improvement was found by continuing the procedure through all except the three or four largest values, which were so large as to cause trouble.

Of the fixed values tested, $s = 2$ gave the most rapid approach to maximum accuracy, although $s = 1$ was also efficient in this respect. A high proportion of the eigenvalues fall in the range $1 \leq s \leq 2$, and thus a value for s would have been chosen in this region if the procedure for selection of s suggested by Peaceman & Rachford had been adopted.

5. CHANGES OF STEP IN THE SPACE VARIABLE

No attempt was made in Phelps' work to use different values of δr in different parts of the range in r. In the earlier investigations by the author [5] it had been noted that, if a change is made in δr, convergence is more rapid if s is kept fixed across the whole range of r than if s is changed in order to give the same value of δt across that range. The problem of change of step in t has been discussed theoretically by Rachford and J. Douglas [18], in connection with Case II in two space variables, but no discussion is given of a change of step in r. It is, of course, analogous to the problem of solution of two similar equations holding it two different media separated by a boundary. This suggests that each region should be analysed separately, equations being set up across the boundaries in some suitable way. For convergence of the whole system we should generally require the B_k in neighbouring regions to be the same and the overall normal modes to be stable. Work on this is being currently pursued in Cambridge by Dr. Iglesias with a view to satisfactory extension of the methods described to more than one space variable.

6. MORE THAN ONE SPACE VARIABLE

Several applications of difference replacement of the forward difference type have been made to equations involving more than one space variable, both for Case II and for Case I. The most usual approach to Case I is to use the Liebmann method [19], or to adopt a process of relaxation [20]. These procedures have mainly been applied to Laplace's equation. In this case we write for the Liebmann method:

$$V(x_i,y_j,t_{k+1}) = \tfrac{1}{4}\Big\{ V(x_{i+1},y_j,t_k) + V(x_{i-1},y_j,+t_k) + V(x_i,y_{j+1},t_k) + V(x_i,y_{j-1},t_k)\Big\}$$

where the introduction of the variable t is usually acknowledged only implicitly. Subtracting $V(x_i,y_j,t_k)$ from each side, we see that this is an example of Case I with $\delta t/\delta x^2 = \delta t/\delta y^2 = \tfrac{1}{4}$. It can be shown that $\tfrac{1}{4}$ is the maximum value that each may assume for stability.

It has been shown by J.Douglas [21] that a stable process can be found in the form

$$\Delta_0 w = (\delta t/\delta x^2)\,\delta^2_{0x} w + (\delta t/\delta y^2)\,\delta^2_{1y} w, \text{ where } \Delta_0 w = w(x_i,y_j,t_{k+1}) - w(x_i,y_j,t_k),$$

$$\delta^2_{kx} w = w(x_{i+1},y_j,t_k) - 2w(x_i,y_j,t_k) + w(x_{i-1},y_j,t_k), \text{ and similarly for } \delta^2_{ky}.$$

For this procedure there is no restriction on the values of $\delta t/\delta x^2$, $\delta t/\delta y^2$. This method has been applied in practice by Peaceman & Rachford [16]. with success, but the grid on (x,y) had equal intervals in each variable. The problem of what boundaries to use when changing step in x or y has not yet been satisfactorily solved.

Apart from the simplest replacement procedures, using small steps in t and a large number of points over the space grid, no applications in more than two variables are known to the author. An application to three variables of direct Liebmann methods which yielded interesting results has been made by Bartlett[22]. in solving the Helium equation. The resulting accuracy, however, is very low. It is felt that more sophisticated methods can be derived by extension of the processes described here, and that these will make it possible to reduce greatly the work required to obtain a given accuracy.

1. Crank, J. 'Mathematics of Diffusion' , Oxford, 1956.

2. Hartee, D.R. Private communication.

3. King, G.W. Tech. Rep. No.4. O.N.R. Project NR033, 243, U.S.A., 1950.

4. see, e.g. Kemble, E.C. 'The Fundamental Principles of Quantum Mechanics' McGraw-Hill, 1937.

5. Douglas, A.S. Thesis for the degree of Ph.D., Cambridge University, 1954.

6. Young, D.M. Trans. Amer. Math. Soc. 75, 92, 1954.

7. Collatz, L. 'Numerische Behandlung von Differentialgleichungen' Springer, 1955.

8. Crandall, S.H. Quart. Appl. Math. 13, 318, 1955.

9. O'Brien, G.G., Hyman, M.A., and Kaplan, S.A. J. Math. Phys. 29, 223, 1951.

10. Crank J. Nicholson, P. Proc. Camb. Phil. Soc. 43, 50, 1947.

11. Juncosa & Young, D.M. (a) Proc. Camb. Phil. Soc. 53, 448, 1957.
(b) Proc. Amer. Math. Soc. 5, 168, 1954.
(c) J. Soc. Indust. Appl. Math. 1, 111, 1953.

12. Milne, W.E. 'Numerical Solution of Differential Equations' John Wiley, New York, 1953.

13. Frankel, S.P. and DuFort, E.C. M.T.A.C. VII, 43, 135, 1953.

14. Richardson, L.F. Phil. Trans. Roy. Soc. 242, 439, 1950.

15. Leigh, D.C.F. Thesis for the degree of Ph.D., Cambridge University, 1955.

16. Peaceman, D.W. and Rachford, H.H. J. Soc. Indust. Appl. Math. 3, 28, 1955.

17. Phelps, J. Dissertation for the Diploma in Numerical Analysis, Cambridge University, 1956.

18. Douglas, J. and Rachford, H.H. Trans. Amer. Math. Soc. 82, 421, 1956.

19. Liebmann, H. Sitzungsber. Bayer. Akad. Munchen, 385, 1918.

20. Southwell, R.V. 'Relaxation Methods in Theoretical Physics', Oxford, 1946.

21. Douglas, J., J. Soc. Indust. Appl. Math. 3, 42, 1955.

22. Barlett, J.H. (a) Phys. Rev. 88, 525, 1952.
(b) Phys. Rev. 98, 1067, 1955.