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A NOVEL FINITE DIFFERENCE FORMULATION FOR DIFFERENTIAL EXPRESSIONS INVOLVING BOTH FIRST AND SECOND DERIVATIVES

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SUMMARY

It is shown that the upwind difference scheme of formulating differential expressions, in problems involving transport by simultaneous convection and diffusion, is superior to the central difference scheme, when the local Peclet number of the grid is large. Even better schemes are derived and discussed. It is pointed out that the best finite difference analogues are found by approximating differential expressions as a whole, and that simple (e.g. one-dimensional) exact solutions form a useful, legitimate and independent source of these optimum algebraic formulae.

INTRODUCTION

The problem considered

There are many ways in which sets of algebraic equations can be constructed so as to simulate, in major respects, the behaviour of partial differential equations; but some ways are better than others in accuracy of simulation, convenience in use, and tendency to promote convergence in iterative solution procedures. Since engineers are increasingly concerned with obtaining solutions to differential equations by numerical means, rules are needed for the best ways of formulating the corresponding algebraic equations in particular circumstances.

In order to predict processes involving the flow of heat and matter, the engineer must solve elliptic, parabolic or hyperbolic differential equations in which appear both first and second derivatives of the main dependent variable, usually with non-constant coefficients; he must often therefore select finite difference analogues of these derivatives. The present paper is concerned with which of the various possibilities is the best, from various points of view.

The present contribution

Although the problem has many aspects and can be treated at great length, some useful results can be established by concentrating attention on a very simple version of the problem, and then generalizing the conclusions. Of course the generalized conclusions will need verification, either by way of a numerical experiment or by means of a higher level analysis. An example of the former is provided by Runchal[1] in a companion paper.

Attention will be concentrated on the formulation of the difference equations for a grid comprising at most three points, all located on a straight line; variability of coefficients will be dispensed with, and we shall consider a differential equation having just one first derivative and one second derivative. It will be shown that the conventional Taylor-series-expansion procedure leads to finite-difference equations which are seriously deficient in accuracy. The so-called 'upwind difference' formula proves to be better over the greater part of the range of conditions,

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but there is a range in which it is actually inferior to the conventional formula. These findings naturally suggest a search for a new formula which combines the best features of both formulations. Such a formula is presented here.

ANALYSIS

The mathematical problem

Let us consider the steady-state transfer of heat in a one-dimensional moving medium, without internal heat sources [Figure 1(a)]. The differential equation governing the variation of temperature T with distance x is

$$c_p G\frac{\mathrm{d}T}{\mathrm{d}x}-\lambda\frac{\mathrm{d}^2 T}{\mathrm{d}x^2}=0 \tag{1}$$

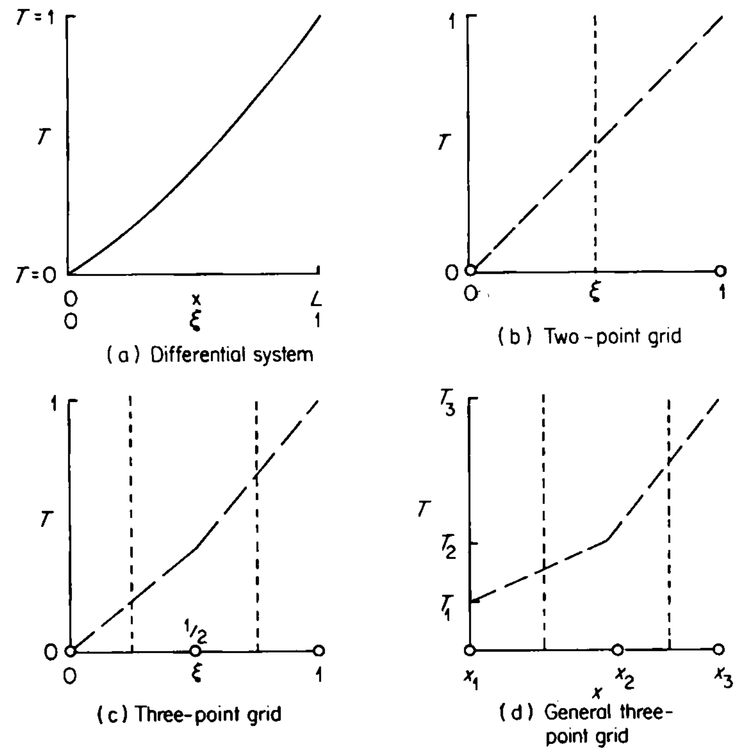

Figure 1. Illustrations of the situations considered.

where c_p stands for the constant-pressure specific heat, G for the mass flow rate of material per unit cross-sectional area in the positive-x direction, and λ for the thermal conductivity of the medium. To emphasize its main features, we can rewrite the equation as

$$P\frac{\mathrm{d}T}{\mathrm{d}\xi}-\frac{\mathrm{d}^2 T}{\mathrm{d}\xi^2}=0 \tag{2}$$

where P stands for the Peclet number, i.e. the non-dimensional quantity $c_p GL/\lambda$; L is the length of the domain of interest; and ξ is the length ratio x/L. We see that P controls the relative importance of the first-order and second-order terms.

Let us further suppose that the temperatures of the boundaries of the one-dimensional domain are held at zero and at unity respectively (obviously, the units in which temperature is measured are immaterial). Then the boundary conditions may be expressed as:

$$\xi = 0: \quad T = 0 \tag{3}$$

$$\xi = 1: \quad T = 1 \tag{4}$$

Our task is to obtain the solution of the equation with these boundary conditions, by means of various finite difference procedures. Comparison with the exact solution will then enable us to discriminate between the procedures.

The exact solution

It is easy to establish that the general solution of our problem is:

$$T = A\,\mathrm{e}^{P\xi} + B \tag{5}$$

where A and B are arbitrary constants. Insertion of the boundary conditions into equation (5) leads to

$$\xi = 0: \quad 0 = A + B \tag{6}$$

$$\xi = 1: \quad 1 = A\,\mathrm{e}^{P} + B \tag{7}$$

Hence

$$A = 1/(\mathrm{e}^{P} - 1) \tag{8}$$

and

$$B = -1/(\mathrm{e}^{P} - 1) \tag{9}$$

The required solution is therefore

$$T = (\mathrm{e}^{P\xi} - 1)/(\mathrm{e}^{P} - 1) \tag{10}$$

Its nature is illustrated by Figure 2, which shows $T \sim \xi$ distributions for various values of P. Inspection shows that T lies always within the extreme values 0 and 1. When P becomes very large and positive, the $T \sim \xi$ curve is nearly horizontal at zero, with a steep rise as ξ approaches unity; when P is large and negative, the horizontal part lies near unity and the steep part near $\xi = 0$.

It will be interesting later to enquire as to the net transfer of energy across the mid-plane of the domain, to which we ascribe the symbol $Q_{\frac{1}{2}}$. This is given by:

$$Q_{\frac{1}{2}} = Gc_p T_{\frac{1}{2}} - \lambda \left(\frac{\mathrm{d}T}{\mathrm{d}x}\right)_{\frac{1}{2}} \tag{11}$$

Insertion of equation (10) leads to

$$(Q_{\frac{1}{2}} L)/\lambda = -P/(\mathrm{e}^{P} - 1) \tag{12}$$

When $|P|$ is very small, the expression on the right hand side tends to -1; this is the value appropriate to the transfer of heat by conduction only. When $|P|$ is very large and positive the non-dimensional heat flux $Q_{\frac{1}{2}} L/\lambda$ is zero; when P is very large in magnitude, but negative, the non-dimensional heat flow to the right is P.

A satisfactory finite difference analogue of the differential equation will display all the above-mentioned features. Some quantitative difference is perhaps inevitable; but this must diminish to an arbitrarily small magnitude when the grid is progressively refined.

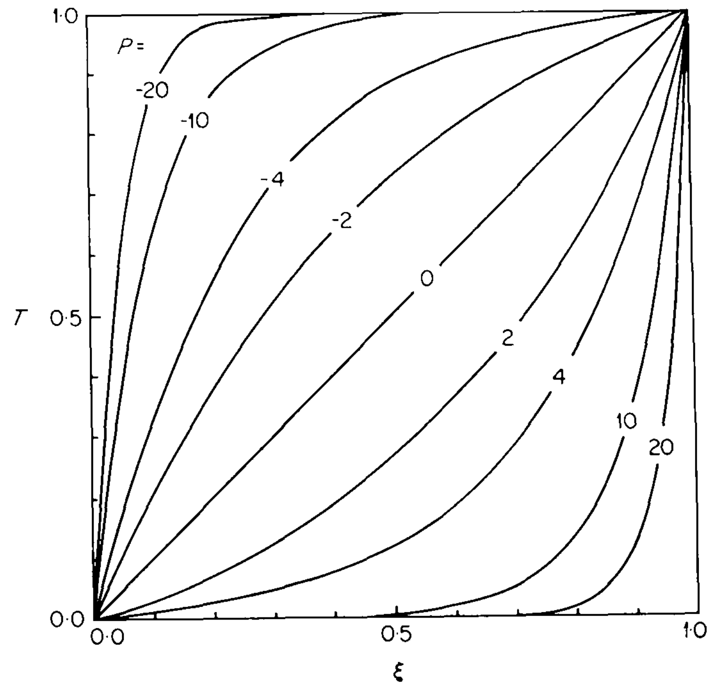

Figure 2. $T \sim \xi$ curves according to equation (10) for various values of P

Solution by central difference scheme (CDS)

It will be simplest, and quite adequate, to consider a grid having either two or three points in the domain of interest. Let us first consider a grid with points at $\xi = 0$ and $\xi = 1$ only [Figure 1(b)], and investigate the transfer of energy across the plane which intersects the ξ-axis normally at $\xi = \frac{1}{2}$. This investigation is important, because, when a multi-point grid is used in the analysis, it is often convenient to surround each grid point with its own plane-faceted volume element, and to determine the temperature which prevails at the grid point by placing equal to zero the sum of the energy fluxes through the individual facets.

The central difference scheme of finite differencing, which is based on a severely truncated Taylor series expansion, implies that the temperature profiles are linear between grid points. The consequence is

$$Q_{\frac{1}{2}} = Gc_p \tfrac{1}{2}(0+1) - \lambda(1-0)/L$$

that is,

$$(Q_{\frac{1}{2}} L)/\lambda = \tfrac{1}{2}P - 1 \tag{13}$$

It is interesting to note that, if the exact expression on the right of equation (12) is expanded and truncated, it implies

$$\begin{aligned}(Q_{\frac{1}{2}} L)/\lambda &\approx -P/[P(1+\tfrac{1}{2}P)] \\ &\approx -1+\tfrac{1}{2}P \end{aligned} \tag{14}$$

Therefore the CDS agrees with the exact solution for P close to zero.

When P is large and positive, $(Q_{\frac{1}{2}} L)/\lambda$ tends to $\frac{1}{2}P$, instead of zero; and at the other extreme it tends to $\frac{1}{2}P$ instead of P. These disagreements are rather severe.

In order to exhibit the influence of the CDS on the calculation of temperature (as distinct from energy flux), we must introduce a third point to our grid [Figure 1(c)]. Let this be at $\xi = \frac{1}{2}$; and let our problem be that of determining the temperature that prevails there. The conventional CDS analogue to the differential equation (2) is

$$\frac{P(T_1 - T_0)}{(\xi_1 - \xi_0)} - \frac{T_1 + T_0 - 2T_{\frac{1}{2}}}{\{\frac{1}{2}(\xi_1 - \xi_0)\}^2} = 0 \tag{15}$$

wherein, for clarity, we have introduced the symbols T_0, ξ_0 and T_1, ξ_1 for the appropriate values at the two grid points, 0 and 1. Hence:

$$P - \frac{(1 - 2T_{\frac{1}{2}})}{1/4} = 0 \tag{16}$$

and so

$$T_{\frac{1}{2}} = \tfrac{1}{2}(1 - P/4) \tag{17}$$

The relation of this solution for the mid-point temperature to the exact one, namely:

$$T = (e^{P/2} - 1)/(e^{P} - 1) \tag{18}$$

may be seen by expanding and truncating the latter. The result is:

$$T = \frac{P/2 + \frac{1}{2}(P^2/4) + \ldots}{P + \frac{1}{2}P^2 + \ldots}$$

$$\approx \tfrac{1}{2}(1 - P/4) \tag{19}$$

Thus the CDS solution agrees with the exact one at small values of $|P|$. However, when P tends to $+\infty$, $T_{\frac{1}{2}}$ tends to $-P/8$ instead of 0, the value appropriate to the exact solution; and as P tends to $-\infty$, $T_{\frac{1}{2}}$ tends to the same expression, whereas the exact solution is unity. These are very serious differences.

Solution by upwind difference scheme (UDS)

Most of the authors who have been successful in devising generally valid solution procedures for problems of fluid dynamics, have employed a procedure which is often termed the 'upwind difference' scheme. This is a scheme which implies that, in the present terms, the fluid crossing an interface possesses the temperature prevailing at the last grid point which it passed; another implication is that $(\mathrm{d}T/\mathrm{d}\xi)_{\frac{1}{2}}$ is approximated by $(T_{\frac{1}{2}} - T_0)/(\xi_{\frac{1}{2}} - \xi_0)$ when P is positive (i.e. the 'wind' blows from ξ_0 to $\xi_{\frac{1}{2}}$) and by $(T_1 - T_{\frac{1}{2}})/(\xi_1 - \xi_{\frac{1}{2}})$ when P is negative.

The resulting expression for the heat flux across the mid-plane of the two-point grid is

$$P \geqslant 0: \quad (Q_{\frac{1}{2}} L)/\lambda = -1 \tag{20}$$

$$P \leqslant 0: \quad (Q_{\frac{1}{2}} L)/\lambda = P - 1 \tag{21}$$

This solution is represented, along with the corresponding lines for the central difference formula and for the exact solution, in Figure 3. It is evident that the UDS agrees with the other two when P equals zero; for $|P|$'s of moderate value, the UDS lines are farther from the exact curve than is the CDS line; but when $|P|$ is large, the UDS solution is more exact than the CDS one.

It is easy to derive the corresponding solution for $T_{\frac{1}{2}}$ of the three-point grid. It is

$$P \geqslant 0: \quad \frac{P(T_{\frac{1}{2}} - T_0)}{(\xi_{\frac{1}{2}} - \xi_0)} - \frac{T_1 + T_0 - 2T_{\frac{1}{2}}}{\{\frac{1}{2}(\xi_1 - \xi_0)\}^2} = 0$$

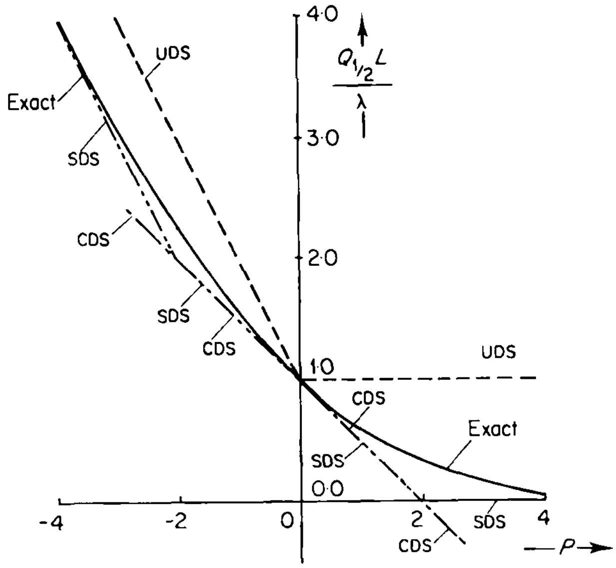

Figure 3. Dependence of dimensionless energy flux across the $\xi = \frac{1}{2}$ plane on the Peclet number P, according to the exact solution, equation (12), and to three finite difference schemes

that is,

$$T_{\frac{1}{2}} = \tfrac{1}{2}/(1+P/4) \tag{22}$$

$$P \leqslant 0: \quad \frac{P(T_1 - T_{\frac{1}{2}})}{(\xi_1 - \xi_{\frac{1}{2}})} - \frac{T_1 + T_0 - 2T_{\frac{1}{2}}}{\{\frac{1}{2}(\xi_1 - \xi_0)\}^2} = 0$$

that is,

$$T_{\frac{1}{2}} = \frac{1}{2}\frac{(1-P/2)}{(1-P/4)} \tag{23}$$

The curves corresponding to equations (22) and (23) are plotted in Figure 4, along with the curves representing the CDS solution [equation (17)] and the exact solution [equation (18)]. It can be seen that, although the agreement of the CDS line with the exact curve is slightly better for moderate values of $|P|$, the agreement of the UDS curve is much better for large values of $|P|$.

DISCUSSION

CDS *or* UDS

Inspection of Figures 3 and 4 shows that the upwind difference scheme, though it shows mild departures from the exact analysis over part of the Peclet number region, is never grossly in error. The central difference formula, on the other hand, becomes quite unrealistic when P lies outside the ranges -2 to $+2$ (for Figure 3) and -4 to $+4$ (for Figure 4).* It is interesting to remark that the limiting values are precisely those which bound the region in which the CDS formula, when employed as a successive-substitution formula in an iterative calculation procedure, leads to convergence. The UDS formula leads to convergence, by contrast, for all values of P.

* The difference in these numbers result from the fact that the grid interval is 1 in the first case and $\frac{1}{2}$ in the second. In physical terms the limiting value is $Gc_p\,\delta x/\lambda = 2$ in both cases, where δx is the distance between grid points.

This finding is worthy of emphasis; for it is sometimes asserted that the upwind scheme, by reason of its lack of symmetry, is always less accurate than the central difference one. This assertion is very remote from the truth. By preferring the UDS to the CDS for large $|P|$, one benefits in respect of both accuracy *and* convergence.

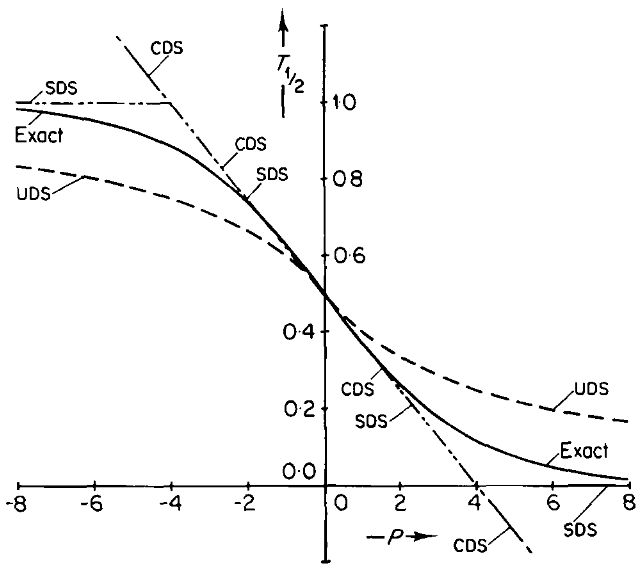

Figure 4. Dependence of the mid-point temperature $T_{\frac{1}{2}}$ on the Peclet number according to the exact solution, equation (18), and to three finite difference schemes

Before leaving this matter, it is perhaps worth remarking that finite-difference equations can also be derived for equations such as (2) by the application of the calculus of variations.[2] Such an application, in which the first-order differential coefficient is treated as a constant, leads to precisely the same formula as is yielded by Taylor-series expansion. Our strictures on the CDS can thus be applied also to the variational formula.

Improved formulae

Inspection of Figures 3 and 4 shows that we can easily devise a formula that is better than the UDS. The best of all would of course be the exact solution itself; interpreting this as a finite difference expression, we should proceed thus:

1. From equation (12), modified so as to refer to the energy flux $Q_{1\frac{1}{2}}$ across the mid-plane separating two locations x_1 and x_2 (Figure 1(d)), we deduce

$$Q_{1\frac{1}{2}} = \frac{Gc_p(T_1-T_2)}{\exp\left[Gc_p(x_2-x_1)/\lambda\right]-1}+Gc_p T_1 \tag{24}$$

Similarly, the energy flux across the plane between x_2 and x_3 is

$$Q_{2\frac{1}{2}} = \frac{Gc_p(T_2-T_3)}{\exp\left[Gc_p(x_2-x_1)/\lambda\right]-1}+Gc_p T_2 \tag{25}$$

2. By equating these two quantities, which implies making an energy balance for the volume bounded by the two mid-planes, we easily deduce

$$T_2 = \frac{T_1(1+f_1)+T_3 f_3}{1+f_1+f_3} \tag{26}$$

where

$$f_1 \equiv \{\exp[Gc_p(x_2-x_1)/\lambda]-1\}^{-1} \tag{27}$$

$$f_3 \equiv \{\exp[Gc_p(x_3-x_2)/\lambda]-1\}^{-1} \tag{28}$$

Equation (26) can be used as the algebraic formula from which T_2 can be deduced when T_1 and T_3 are given. Obviously, the arguments of f_1 and f_3 can differ; so the formula is useful for grid spacings, thermal conductivities and even mass flow rates, which are non-uniform.

The most significant feature of equation (26), from the standpoint of the developer of numerical solution schemes for differential equations, is perhaps that the expressions for the f's are derived from a *solution* of the differential equation.

It may be thought that, if the solution is available, there is no need for the use of a difference scheme at all. The countering point to remember is that these same expressions for the energy fluxes can be advantageously used for setting up the energy balance for a point in a *two*-dimensional grid. For a two-dimensional problem, the exponential form of profile is of course not, in general, the exact solution. However, one might just as well employ a finite difference formula which reduces to the exact solution sometimes rather than one which never does so.

Exponential functions are time-consuming to compute. It would therefore be foolish to advocate the employment of equation (26) in a finite difference calculation procedure until it has been clearly demonstrated that its increased potential accuracy is not more economically gained by the use of a finer grid. To investigate this question would be a simple exercise, but it has not so far been carried out.

In the meantime, simpler formulae can be devised. Perhaps the simplest of all (designated SDS in Runchal's paper[1]), is a combination of the CDS and UDS ideas. It can be expressed by means of the equations for $Q_{\frac{1}{2}}$:

$$-2 \leqslant P \leqslant 2: \quad (Q_{\frac{1}{2}}L)/\lambda = \tfrac{1}{2}P - 1 \tag{29}$$

$$P > 2: \quad (Q_{\frac{1}{2}}L)/\lambda = P \tag{30}$$

$$P < -2: \quad (Q_{\frac{1}{2}}L)/\lambda = 0 \tag{31}$$

The corresponding straight lines are marked on Figure 3; Figure 4 carries the corresponding solution for $T_{\frac{1}{2}}$ in the three-point-grid problem. Evidently this prescription is somewhat more accurate, over-all, than the UDS one, and it also happens to keep the finite difference coefficients within bounds that ensure convergence.

It is not difficult to devise simple formulae that fit the exact solution even more closely, without involving three separate parts, and without employment of exponential or similar functions. However, only that represented by the above three equations has actually been put to the test so far.[1] It proves to be significantly superior to both the CDS and the UDS for the problem investigated there.

Final remarks

It is foolhardy for an untrained amateur of numerical analysis to propose a novel principle in this highly developed subject. Nevertheless, the foregoing investigation focuses attention on two aspects of finite difference practice that may yield further fruit and that seem to be not often considered. The first is that there is no 'best formulation' for a first-derivative or second-derivative expression *in isolation*: it is the combination of the first and second derivatives, as they appear in a particular differential equation, that require to be represented by an algebraic expression; and the best form for this expression depends on the relative magnitude of the two terms.

The second point is that finite difference expressions can be usefully constructed so as to fit exactly, or almost exactly, the true solution of the differential equation under simple circumstances. This practice is quite distinct from, for example, derivation by Taylor-series expansion, and it seems to be much more satisfactory. Many extensions of this principle can be envisaged.

The writer would be interested to learn of earlier explicit or implicit statements of these principles.

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REFERENCES

1. A. K. Runchal, 'Convergence and accuracy of three finite difference schemes for a two-dimensional conduction and convection problem', *Int. J. num. Meth. Engng*, **4**, 541–550 (1972).
2. M. Hiroaka and K. Tanaka, 'A variational principle for transport phenomena', in *Memoirs of Faculty of Engineering*, Part 3, Kyoto University (1968), pp. 235–263.