SHORT COMMUNICATION A NOTE ON THE STEADY-STATE ADVECTION–DIFFUSION EQUATION

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SUMMARY

In this note we show that the numerical solution of the advection-diffusion equation can be improved by considering the asymptotic behaviour of its analytical solution. This is accomplished by including a correction term based on the numerical differentiation of the asymptotic ($Pe \gg 1$, Pe being the Peclet number) solution. This correction forces the usual oscillations associated with centred schemes to disappear.

BACKGROUND

Let us assume that we are trying to find the solution for a problem

$$L(u) = 0. \tag{1}$$

by means of a discrete technique. Here, L represents a differential operator which we assume to be linear, elliptic and homogeneous. The non-homogeneous case can be treated similarly.

Let the discrete version of equation (1) be represented by

$$L_h(U) = 0. \tag{2}$$

Then, a possible iterative scheme for the numerical solution of (2) is

$$(I - kL_h)U^{n+1} = U^n - kL_h(F).$$
(3)

Equation (3) constitutes a 'fully implicit' approximation to equation (2) when $L_h(F) = 0$, and can be considered as a pseudo-non-steady algorithm. In this equation I is the identity operator and k is the 'time step'.

Let us consider the last term of equation (3). Suppose for a moment that F is the analytical solution of equation (1). Then, if L_h is an exact representation of (1) (i.e. without any truncation error), then $L_h(F) = 0$. The exact representation of a differential operator cannot be used in practice and $L_h(F) \neq 0$. Now, if equation (3) is considered as the discrete representation for the numerical solution of (1) and $U^n \rightarrow U^{n+1} \rightarrow U$ for a high enough n, then

$$L_h(U-F)=0.$$

If we assume that L_b does not annihilate U - F, then $U \equiv F$, which is an interesting (and obviously

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expected) result. However, this does not naturally occur; instead, the converged result with actually satisfy

$$L_h(U) = L_h(F).$$

The role of the last term of equation (3) can now be made clear: it can provide a link between the computed solution and a known behaviour of the solution of equation (1). In many cases of physical interest, the solution of the governing equation (1) shows a boundary layer behaviour, and the usual discrete approximations often fail. The case of the solution of Burgers' equation, with an outflow boundary layer, is a common example. The reason for the failure of the discrete representations usually lies in their poor resolution, within the boundary layer. In what follows we consider the improvement of the accuracy of the discrete solution of (1) for a given grid by means of a suitable specification of F, in connection with the *a priori* knowledge of the asymptotic behaviour of the solution of (1).

Then, the basis for the specification of a linking function should be related to the asymptotic behaviour of the solution of equation (1).

As can be seen from equation (3), the effect of $L_h(F)$ consists in the spreading of the truncation error of the discrete representation of L over all the grid points. To a certain extent, the present approach resembles Emery's technique¹, which he employed for the proper treatment of singularities of heat generation in continuous media.

In Emery's technique the singularities exist and they originate a strong variation of the dependent variable (a boundary layer). In the present technique we added a distributed, fictitious source to account for the boundary layer behaviour of the solution, if there is any. Both methods have a common feature in the sense that L_h must be a good approximation for *L* outside the boundary layer.

In order to specify the problem (3), we must define the order of the approximation of L_h . In the following, a three-point, second-order, space-centred approximation is considered for all cases. In the case of first-order derivatives, we employ Lagrange's formula to evaluate the derivative at the central point (to account for the case in which the grid is variable). This formula reduces to the usual centred space approximation for constant grid spacing.

In what follows, we show the advantages of incorporating the knowledge of the asymptotic behaviour of the solution into the computational algorithm. The example shown is limited in scope but is representative of the concept involved.

THE STEADY ADVECTION-DIFFUSION EQUATION

This is the case considered in References 2-5, and is sometimes called the 'tough' problem, namely

$$-Pe u' + u'' = 0; u(0) = 0, \quad u(1) = 1, \tag{4}$$

where the primes indicate differentiation with respect to the space co-ordinate x, Pe = VL/D is the Peclet number V is the constant transport velocity, L is length of the integration domain and D is the diffusivity. This problem is interesting because, if a centred discrete scheme is employed in the numerical representation of (4), there exists a limiting grid Peclet number beyond which the exact numerical solution of (4) becomes oscillatory (see References 2–5 for a detailed discussion of this behaviour).

The case of interest here is considering a fixed number of space increments and a high enough Pe, so as to force the 'knee' of the solution into the last space interval. It is well known³ that the numerical solution is, in this case, oscillatory.



Figure 1. Comparison of computed and analytical solutions for the advection-diffusion equation.----: analytic solution; black symbols: corrected iterative solution; open symbols: standard iterative solution; b&w symbols: coincident computed results

The approximate analytical solution of (4), for a high Pe, can be written as follows:

$$F(x) = e^{-Pe(1-x)}.$$
 (5)

(The exact solution is

$$F(x) = \frac{1 - e^{Pex}}{1 - e^{Pe}}.$$

Let us now consider the results so obtained. Figure 1 shows the solutions for several values of Pe, employing 10 space intervals (we denote the space interval as h from here on). Then h = 0.1. By simply setting F as zero in the computer code, the results of the standard iterative technique may be obtained. For low Pe, the two techniques give identical results. As Pe increases the results obtained with the corrected iterative technique are much better than the ones obtained with the standard technique.

The corrected iterative technique also works very well for $Pe = 10^4$, 10^5 and infinity, showing very slight oscillations (of the order of 10^{-12} in every node). Of course, no one should ask for such a solution with this small number of nodes and constant spacing; nevertheless, the computed results are interesting.

The case with Pe = 60 is of particular interest because the 'knee' reaches the last interval. In this case the computed result ($u = 0.674 \times 10^{-2}$ for x = 0.9) is coincident with the analytical result to three significant digits. It is worth mentioning that the results discussed above supply a better

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approximation than the ones obtained by means of the Galerkin method with a finer grid (see Reference 2, chapter 5).

The results shown above can be explained in terms of the exact algebraic solution of equation (3), assuming that convergence to 'steady state' has been achieved. If we approximate equation (4) by means of centred differences, as stated above, then the solution of the difference equation is⁵

$$e_m = U_m - F_m = C_1 z^m + C_2, (6)$$

where

$$z = (1 + \theta)/(1 - \theta); 2\theta = Pe/M; M = h^{-1}.$$

The integration constants C_1 and C_2 are determined considering that F does not necessarily satisfy the boundary conditions imposed by equation (4). In fact, from (5), $F(0) = \exp(-Pe)$. Then

$$e_0 = -\exp(-2M\theta); e_M = 0.$$

After determining C_1 and C_2 from the given boundary conditions, equation (6) becomes

$$e_m = e^{-Pe} z^M \left\{ \frac{1 - z^{m-M}}{1 - z^M} \right\}.$$
 (7)

Now the behaviour of the solution of (4) with the present technique can be explained. If we assume that the grid Peclet number is small as compared with M, then

$$U_m \equiv e^{-Pe(1-x)} + (x-1) \left[1 + \frac{Pe}{2}(x-1) \right] / \left(1 + \frac{Pe}{2} \right).$$
(8)

If Pe = 0, then $U_m = x$, which is coincident with the analytical solution. When Pe < 0.5 and M = 10, the error of equation (8) with respect to the analytical solution is lower than 10^{-3} over all the grid nodes.

On the other hand, when $Pe \to \infty$, $e_0 \cong 0$ and $e_M = 0$; then $e_m = 0$ and the solution tends to be coincident with equation (5). It must be remembered that the boundary conditions, as shown in (4), still hold for u.

CONCLUSIONS

We have shown that the numerical solution of a particular, although important, problem can be improved by simply considering our knowledge of the asymptotic behaviour of the analytical solution. This is also the case for many important problems in computational physics, and research is now underway in this field. Some preliminary experiments with Burgers' equation, employing a linearized operator, resulted in similar trends. The aim of future work is improving the behaviour of the numerical solution of the Navier–Stokes equations in the vicinity of a wall, particularly the case of very high Raleigh numbers (i.e. $> 10^7$) for free convective flows.

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