INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 13, 739–757 (1991)

DIFFERENTIAL-EQUATION-BASED REPRESENTATION OF TRUNCATION ERRORS FOR ACCURATE NUMERICAL SIMULATION

ROBERT J. MACKINNON AND RICHARD W. JOHNSON

Idaho National Engineering Laboratory, EG&G Idaho, Inc., Idaho Falls, ID 83415-2403, U.S.A.

SUMMARY

High-order compact finite difference schemes for two-dimensional convection–diffusion-type differential equations with constant and variable convection coefficients are derived. The governing equations are employed to represent leading truncation terms, including cross-derivatives, making the overall $O(h^4)$ schemes conform to a 3×3 stencil. We show that the two-dimensional constant coefficient scheme collapses to the optimal scheme for the one-dimensional case wherein the finite difference equation yields nodally exact results. The two-dimensional schemes are tested against standard model problems, including a Navier–Stokes application. Results show that the two schemes are generally more accurate, on comparable grids, than $O(h^2)$ centred differencing and commonly used $O(h)$ and $O(h^3)$ upwinding schemes.

KEY WORDS High-order finite difference method Convection diffusion Upwind differencing Artificial diffusion Navier–Stokes

INTRODUCTION

Many physical systems, especially those involving fluid flow, are described in terms of mathematical models that include convective and diffusive transport of some variable. It is well known that numerical solutions of such model equations can yield spatially oscillatory results. An array of numerical tools, notably various upwinding schemes, has been generated over the years to eliminate such spurious oscillations, albeit often at the expense of accuracy.

Numerical schemes for approximating convection–diffusion equations usually employ centred differencing for the second-order derivative diffusion terms and some form of backward (upwind) differencing for the convection terms. The standard first-order upwind difference scheme (UDS) and the popular third-order upwind scheme of Leonard[1] (herein referred to as LDS) are among them. These and other schemes are categorized and discussed in the reviews by Patel *et al.*[2] and Leschziner.[3]

An alternative approach to backward differencing is to add, directly, an artificial diffusion (dissipation) term to the physical diffusion and use the standard five-point centred difference scheme (CDS). The disadvantage of this technique, as with the UDS scheme, is that it smooths the solution in all directions. (It is well known that this approach is equivalent to the UDS for an appropriate choice of artificial diffusivity.)

It has in fact been demonstrated for a simple one-dimensional convection–diffusion problem that if the proper (optimal) amount of artificial diffusion is added, the numerical solution to the discrete equation will be nodally exact. This fact has motivated *ad hoc* generalizations of the

0271–2091/91/160739–19$09.50

Received 20 February 1990
Revised 16 October 1990

optimal one-dimensional formulation to multidimensions. Generally, these formulations are not optimal and tend to work well only for problems in which the flow is aligned with the grid. In problems that do not conform to this condition, numerical solutions will exhibit excessive diffusion normal to the flow direction (crosswind diffusion). An improvement to the above *ad hoc* schemes is the restriction of artificial diffusion to the streamwise direction (streamline upwinding). This approach requires a tensorial artificial diffusivity rather than a scalar one. The concept of a tensorial artificial diffusivity was independently introduced by Dukowitz and Ramshaw[4] for hyperbolic flows and Hughes and Brooks[5] for elliptic and parabolic flows.

The proper method of determining the optimal magnitudes of the components of the diffusivity tensor for a given problem is still an unresolved issue. Hughes and Brooks[5] estimate the optimal strength in an *ad hoc* manner by essentially averaging the optimal one-dimensional diffusivity for each co-ordinate direction. The approach taken by Dukowitz and Ramshaw[4] is theoretically more appealing in that the diffusivity tensor is obtained directly from a Taylor series expansion. That is, temporal truncation errors are expressed, using the governing differential equation, as spatial errors and then explicitly accounted for in the temporal difference approximation by constructing an appropriate tensorial diffusivity. In effect, some of the truncation errors are themselves approximated in the difference scheme, effectively increasing the order of accuracy from first- to second-order.

The objectives of the present study are to derive two differencing schemes for convection-dominated problems which exhibit the smoothing properties of artificial diffusion and yet maintain high-order accuracy, and to determine their behaviour for some standard test cases. The schemes developed herein conform to a compact nine-point (3×3) stencil (in 2D), allowing them to be applied immediately adjacent to a boundary. The formulation is analogous to the approach of Dukowitz and Ramshaw[4] in that it employs the original differential equation to represent truncation error terms and therefore compensates for them. By using the original model equation to represent truncation terms, higher-order derivatives can be replaced with lower-order derivatives that can be approximated on a compact nine-point stencil. Since truncation terms are represented in the numerical differencing scheme, the order of accuracy of the scheme is increased. Note that the technique is applied to all of the terms appearing in the governing differential equation, providing higher-order accuracy for the entire discrete equation (not just for the convection terms). From another perspective, the appropriate form of the tensorial diffusivity and the optimal magnitude of its components are constructed naturally by the new procedure.

A few researchers have applied the same principle used herein for particular applications while others have arrived at equations identical to ours, albeit via different routes. Abarbanel and Kumar[6] employ the original differential equation to obtain a nine-point (in 2D) spatially $O(h^4)$, temporally $O(h^2)$ scheme for the Euler equations; they also extend it to three dimensions. In an earlier study, Jones *et al.*[7] suggest application of this same principle in deriving an $O(h^4)$ scheme for Poisson's equation used in connection with the method of lines.

In deriving their scheme for a convection–diffusion system having variable coefficients, Gupta *et al.*[8] apply series expansions to the differential equation. After considerable manipulation they obtain a difference equation identical to one of the schemes derived in the present study. Dennis and Wing[9] arrive at a scheme similar to our scheme for the two-dimensional, constant coefficient (linear) case by employing the structure of the exact solution and using a finite difference adaptation of the Taylor–Maclaurin method for solving differential equations. In a later paper, Dennis and Hudson[10] derive the same scheme as in Reference 8 using another approach. They extend and modify the basic method of a class of higher-order compact schemes. This class of schemes employs derivatives of the original dependent variable as dependent variables, requiring boundary conditions for the derivatives. To eliminate this requirement, Dennis and Hudson[10] employ a transformation that involves expanding the exponential of a definite integral of the convective coefficient. The approach followed in the present work is more direct than those cited above, involving straightforward differentiation and simple algebra.

The presentation of this paper is as follows. The procedure is first developed for a non-homogeneous, one-dimensional, constant coefficient problem. A new exact difference formula is obtained which includes an optimal diffusivity and modified source term. The procedure is then rigorously extended to the constant coefficient case in two dimensions. The resulting fourth-order scheme is compared in numerical studies with various existing upwind and higher-order schemes.[1,11] Finally, the treatment of variable coefficients is discussed and an example Navier–Stokes calculation is presented.

FORMULATION OF THE PRESENT APPROACH

Motivation

To motivate the main development presented in this study, we consider the steady convection–diffusion model problem

$$-au_{xx}+cu_x=0, \qquad 0\leqslant x\leqslant 1, \tag{1}$$

$$u(0)=0, \qquad u(1)=1, \tag{2}$$

where a and c are positive constants. Here a is the conductivity, c is the convective velocity and the solution u can represent the concentration of a chemical species, heat, vorticity, etc. The exact solution to (1), (2) is

$$u(x)=\frac{1-\exp(cx/a)}{1-\exp(c/a)}. \tag{3}$$

When $c\gg 1$, the solution $u(x)$ contains a boundary layer near $x=1$.

It is well known that the centred difference solution to this problem is oscillatory if the cell Reynolds number Re_h ($=ch/a$) exceeds a value of two. This phenomenon is illustrated in Figure 1. Here we offer a simple explanation for the cause of these unwanted oscillations for the one-dimensional case.

Let x_{i-1}, x_i, and x_{i+1} be three consecutive grid points. Denote the numerical solution at x_i by $u_{hi}=u_h(x_i)$. The numerical solution for the centred difference approximation at the interior grid point x_i satisfies

$$-\frac{a}{h^2}(u_{hi+1}-2u_{hi}+u_{hi-1})+\frac{c}{2h}(u_{hi+1}-u_{hi-1})=0. \tag{4}$$

In order to illustrate how a centred difference discretization can lead to oscillations, we define

$$S_i^+=\frac{u_{hi+1}-u_{hi}}{h}, \qquad S_i^-=\frac{u_{hi}-u_{hi-1}}{h},$$

which represent forward and backward slopes at point x_i. Introducing the above slopes into (4) and rearranging yields

$$S_i^+\left(\frac{a}{h}-\frac{c}{2}\right)=S_i^-\left(\frac{a}{h}+\frac{c}{2}\right). \tag{5}$$

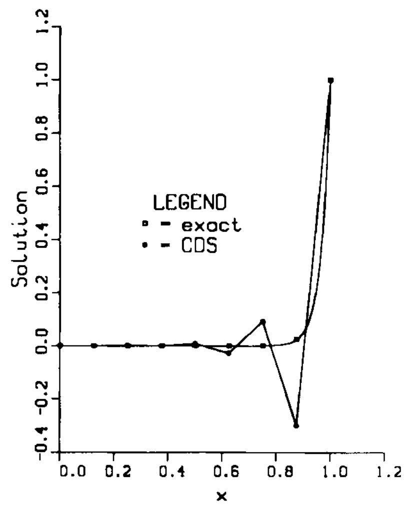

Figure 1. Centred difference scheme (CDS) and exact solutions to a simple 1D convection–diffusion problem (equations (1) and (2)) showing spatially oscillatory behaviour for cell Reynolds number greater than two

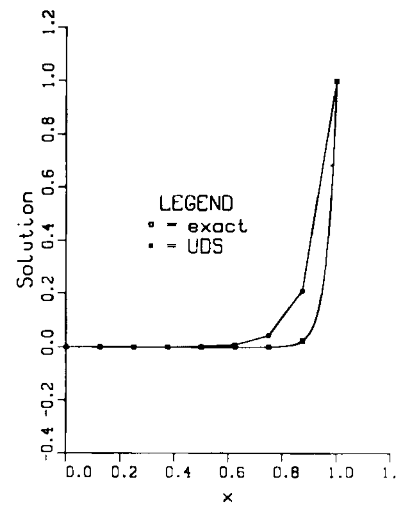

Figure 2. Optimal (exact) and standard upwind (UDS) solutions to the same problem as for Figure 1

Observe that if the cell Reynolds number Re_h exceeds a value of two, S_i^+ and S_i^- must have opposite signs at each x_i. Hence for non-zero u_h, the solution will become oscillatory. Furthermore, for $Re_h=2$, S_i^- and u_{hi} are zero at each interior point, clearly an undesirable result for non-trivial u_h. Only when Re_h is less than two, allowing S_i^+ and S_i^- to have the same sign, is the numerical solution well behaved, increasing monotonically from $x=0$ to $x=1$.

A common approach for suppressing oscillations is to introduce additional diffusion a^* into (4), effectively reducing Re_h. In such a case, (5) would become

$$S^+\left(\frac{a+a^*}{h}-\frac{c}{2}\right)=S^-\left(\frac{a+a^*}{h}+\frac{c}{2}\right). \tag{6}$$

Thus, if a sufficient quantity of artificial diffusion a^* is added to a, the effective cell Reynolds number

$$Re_h^*=\frac{ch}{a+a^*} \tag{7}$$

can be made to have a value less than two. Then the centred difference solution to (1), (2) will be non-oscillatory, though not necessarily accurate. For example, standard upwinding (backward differencing) of the convective term in (1) is equivalent in this case to introducing $a^*=ch/2$, which is known to produce inaccurate results. On the other hand, it can be shown that if the optimal amount of artificial diffusion, $a^*=(ch/2)\coth(ch/2a)$, is added, the centred difference representation to (1) will give exact results at the nodes x_i. The optimal value is determined by introducing the analytical solution (3) directly into the discrete equation (4). Optimal and standard upwind solutions are shown in Figure 2. In the next subsection we present a new approach to developing the optimal upwind difference scheme. This approach does not require the exact solution *a priori*, nor is it restricted to homogeneous problems. Moreover, the methodology extends to problems involving two and three dimensions and variable coefficients.

One-dimensional case

This subsection describes the underlying theory and important features of the proposed method. We begin by developing the approximation for the steady one-dimensional non-homogeneous model problem

$$-au_{xx}+cu_x=f, \qquad 0\leqslant x\leqslant 1, \tag{8}$$

$$u(0)=\gamma_1, \qquad u(1)=\gamma_2, \tag{9}$$

where a and c are constants, $a>0$, and f is a sufficiently smooth function of x.

The domain [0, 1] is uniformly subdivided into N intervals with $x_i=ih$, $h=x_{i+1}-x_i$, $u_i=u(x_i)$, $u_{hi}=u_h(x_i)$ and $i\in\{0, 1, 2, \ldots, N\}$. For a sufficiently smooth solution u, derivatives in (8) at interior grid points x_i, can be defined using Taylor's theorem as

$$D_{xi}u=u_{xi}=D_{hxi}u-\frac{h^2}{3!}D^3_{xi}u-\frac{h^4}{5!}D^5_{xi}u+O(h^6), \tag{10}$$

$$D^2_{xi}u=u_{xxi}=D^2_{hxi}u-\frac{2h^2}{4!}D^4_{xi}u-\frac{2h^4}{6!}D^6_{xi}u+O(h^6), \tag{11}$$

where D^n_{hxi} and D^n_{xi} are the nth-order centred difference operator and the exact derivative operator respectively at x_i.

The key idea in the present development is the following: re-express the high-order derivatives that appear in the Taylor series expansions, equations (10) and (11) in this case, using information given by the original differential equation (8). By so doing, the accuracy of discrete approximation can be increased to arbitrary order (even to exact), since truncation errors pertaining to the discrete operator may be represented in the final discrete equation. For instance, in the case of the centred difference operator for the first derivative, equation (10), the $O(h^2)$ and higher truncation terms can be represented using the original differential equation such that the order of accuracy is increased depending on how many terms are represented. To illustrate this idea, we differentiate (8) to obtain

$$D^3_xu=D_x\left(\frac{1}{a}(cu_x-f)\right)=\frac{c}{a}u_{xx}-\frac{1}{a}f_x, \tag{12}$$

and again to obtain

$$D^4_xu=D_x\left(\frac{c}{a}u_{xx}-\frac{1}{a}f_x\right)=\left(\frac{c}{a}\right)^2u_{xx}-\frac{c}{a^2}f_x-\frac{1}{a}f_{xx}, \tag{13}$$

where (12) has been used to replace the third-order derivative in (13). The nth derivative for this case can be written in the general form

$$D^n_xu=\left(\frac{c}{a}\right)^{n-2}u_{xx}-\sum_{k=1}^{n-2}\frac{c^{k-1}}{a^k}D^{n-k-1}_xf. \tag{14}$$

We now have an expression for the nth-order derivative of u, derived from the differential equation (8), which can be used to represent the derivatives that appear in the Taylor series expansions (10) and (11). Introducing (14) into (10) and (11) and rearranging, we obtain the following relationships between the discrete and exact derivative operators:

$$D_{xi}u = D_{hxi}u - \frac{(c/a)(D^2_{hxi}u + 2\bar{\bar{F}}{}^x_i)S_2}{1 + 2(c/a)^2 S_1} - \bar{F}^x_i, \tag{15}$$

$$D^2_{xi}u = \frac{D^2_{hxi}u + 2\bar{\bar{F}}{}^x_i}{1 + 2(c/a)^2 S_1}, \tag{16}$$

where

$$S_1 = \sum_{n=1}^{\infty} \frac{h^{2n}}{(2n+2)!}\left(\frac{c}{a}\right)^{2n-2}, \tag{17}$$

$$S_2 = \sum_{n=1}^{\infty} \frac{h^{2n}}{(2n+1)!}\left(\frac{c}{a}\right)^{2n-2}, \tag{18}$$

$$\bar{F}^x_i = \sum_{n=1}^{\infty} \frac{h^{2n}}{(2n+1)!} \sum_{k=1}^{2n-1} \frac{c^{k-1}}{a^k} D^{2n-k}_{xi} f, \tag{19}$$

$$\bar{\bar{F}}{}^x_i = \sum_{n=1}^{\infty} \frac{h^{2n}}{(2n+2)!} \sum_{k=1}^{2n} \frac{c^{k-1}}{a^k} D^{2n-k+1}_{xi} f. \tag{20}$$

We find that for this problem we can write S_1 and S_2 in closed form as

$$S_1 = \left(\frac{a}{c}\right)^4 \frac{1}{h^2}\left[\cosh\frac{ch}{a} - \frac{1}{2}\left(\frac{ch}{a}\right)^2 - 1\right], \tag{21}$$

$$S_2 = \left(\frac{a}{c}\right)^3 \frac{1}{h}\left(\sinh\frac{ch}{a} - \frac{ch}{a}\right). \tag{22}$$

Substituting (15) and (16) into (8), using (21) and (22) and simplifying, we obtain

$$-\frac{ch}{2}\coth\left(\frac{ch}{2a}\right) D^2_{hxi}u + cD_{hxi}u = f_i + ch\coth\left(\frac{ch}{2a}\right)\bar{\bar{F}}{}^x_i + c\bar{F}^x_i. \tag{23}$$

Equation (23) is an exact discrete representation of the model transport problem. Observe that when $f(x) = 0$, (23) reduces to the well-known 'exact' (optimal upwind) centred difference representation of the homogeneous transport problem discussed earlier (equations (1) and (2)). Here, however, the analytic solution is not required *a priori* as it was previously.[12]

Remarks. This method may also be applied to more general two-point boundary value problems having sufficiently smooth solutions. If a boundary flux is specified as data, say $-au_x(1) = \Gamma$, a higher-order compact difference formula for Γ can be derived using the procedure outlined above. This formula can be used to discretize the boundary condition in constructing the full set of difference equations for the Neumann problem. This idea is discussed in the context of finite difference and finite element methods by MacKinnon and Carey.[13,14]

In practice it may be more convenient or even necessary to use nodal values for f rather than analytic functions. If the evaluations of $\bar{\bar{F}}{}^x_i$ and $\bar{F}^x_i$ are restricted to node points x_{i-1}, x_i and x_{i+1}, then (23) will be exact for constant or linear f. Otherwise, (23) is formally $O(h^4)$-accurate when f is only given discretely.

Two-dimensional case

In this subsection we extend the one-dimensional formulation to two dimensions. Consider the boundary value problem

$$-(au_{xx}+bu_{yy})+cu_x+du_y=f(x,y), \tag{24}$$

where a, b, c and d are constants, $a, b>0$, and f is sufficiently smooth. Here attention is restricted to regions which may be partitioned into square subregions by a uniform grid. A representative nine-point mesh stencil centred at interior node (x_i, y_j) is shown in Figure 3.

Again, the technique of using the governing equations to represent higher-order derivatives in Taylor series expansions will be used. That is, differentiating (24) once and solving for the third-derivative operator, we get

$$D_x^3u=-\frac{b}{a}D_y^2D_xu+\frac{c}{a}D_x^2u+\frac{d}{a}D_xD_yu-\frac{1}{a}D_xf. \tag{25}$$

Differentiating (24) twice and substituting (25) for the third-order derivative gives

$$D_x^4u=\left(\frac{c}{a}\right)^2D_x^2u+\frac{cd}{a^2}D_xD_yu-\frac{cb}{a^2}D_y^2D_xu+\frac{d}{a}D_yD_x^2u-\frac{b}{a}D_y^2D_x^2u-\frac{1}{a}D_x^2f-\frac{c}{a^2}D_xf. \tag{26}$$

Continuing this process leads to a relationship for the nth derivative of u based on the original differential equation:

$$D_x^nu=\left(\frac{c}{a}\right)^{n-2}D_x^2u+\left(\frac{c}{a}\right)^{n-3}\frac{d}{a}D_xD_yu-\left(\frac{c}{a}\right)^{n-3}\frac{b}{a}D_y^2D_xu$$
$$+\sum_{k=1}^{n-3}\left(\frac{c}{a}\right)^{n-k-3}D_x^{(k)}\left(\frac{d}{a}D_yD_xu-\frac{b}{a}D_y^2D_xu\right)-\sum_{k=1}^{n-2}\frac{c^{k-1}}{a^k}D_x^{(n-k-1)}f. \tag{27}$$

Since we are now working in two dimensions, we indicate that the differential operators appearing in (27) apply to point (x_i, y_j). These operators could be represented using the notation $(D_xD_y)_{ij}$. For brevity we use D_xD_{yij} $(=D_yD_{xij})$.

Now recall from (11) that the Taylor series expansion for u_{xxij} is

$$D_{xij}^2u=u_{xxij}=D_{hxij}^2u-\frac{2h^2}{4!}D_{xij}^4u-\frac{2h^4}{6!}D_{xij}^6u+O(h^6).$$

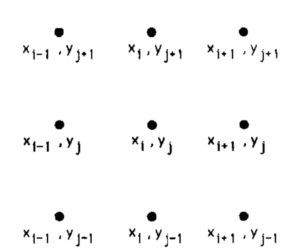

Figure 3. Schematic diagram and nomenclature for the square nine-point differencing stencil used for the 2D schemes derived in the present study

Replacing derivatives $D^4_{xij}u$, $D^6_{xij}u$, etc. using (27) and rearranging, we can rewrite (11) as

$$D^2_{xij}u = D^2_{xhij}u - 2\left[\frac{h^2}{4!}\left(\frac{c}{a}\right)^2 + \frac{h^4}{6!}\left(\frac{c}{a}\right)^4 + \ldots\right]D^2_{xij}u - 2\frac{d}{a}\left[\frac{h^2}{4!}\frac{c}{a} + \frac{h^4}{6!}\left(\frac{c}{a}\right)^3 + \ldots\right]D_x D_{yij}u$$
$$+ 2\frac{b}{a}\left[\frac{h^2}{4!}\frac{c}{a} + \frac{h^4}{6!}\left(\frac{c}{a}\right)^3 + \ldots\right]D^2_y D_{xij}u - 2\frac{d}{a}\left[\frac{h^2}{4!} + \frac{h^4}{6!}\left(\frac{c}{a}\right)^2 + \ldots\right]D_y D^2_{xij}u$$
$$+ 2\frac{b}{a}\left[\frac{h^2}{4!} + \frac{h^4}{6!}\left(\frac{c}{a}\right)^2 + \ldots\right]D^2_y D^2_{xij}u + \bar{\bar{R}}^x_{ij} + 2\bar{\bar{F}}^x_{ij}, \tag{28}$$

where

$$\bar{\bar{R}}^x_{ij} = \sum_{n=6}^{\infty} \frac{h^{n-2}}{n!} \sum_{k=2}^{n-3} \left(\frac{c}{a}\right)^{n-k-3} D^{(k)}_x\left(\frac{d}{a} D_y D_{xij}u - \frac{b}{a} D_x D^2_{yij}u\right) \tag{29}$$

and $\bar{\bar{F}}^x_{ij}$ is given by (20). Equation (28) is an expression that relates the exact derivative to the centred difference operator for the second derivative, with truncation error being represented using the governing differential equation. For convenience we rewrite (28) in the more compact form

$$D^2_{xij}u = D^2_{xhij}u - 2S_1\left[\left(\frac{c}{a}\right)^2 D^2_{xij}u + \frac{dc}{a^2} D_x D_{yij}u - \frac{bc}{a^2} D^2_y D_{xij}u + \frac{d}{a} D_y D^2_{xij}u - \frac{b}{a} D^2_y D^2_{xij}u\right]$$
$$+ 2\bar{\bar{F}}^x_{ij} + \bar{\bar{R}}^x_{ij}, \tag{30}$$

where S_1 is given by (17) and (21). Solving for D^2_{xij} and simplifying, we have

$$D^2_{xij}u = \frac{1}{1 + 2(c/a)^2 S_1}\left[D^2_{xhij}u - 2S_1\left(\frac{dc}{a^2} D_x D_{yij}u - \frac{bc}{a^2} D^2_y D_{xij}u + \frac{d}{a} D_y D^2_{xij}u - \frac{b}{a} D^2_y D^2_{xij}u\right)\right.$$
$$\left. + 2\bar{\bar{F}}^x_{ij} + \bar{\bar{R}}^x_{ij}\right]. \tag{31}$$

A similar procedure is applied to derivative operators $D_{xij}u$, $D^2_{yij}u$, and $D_{yij}u$. The resulting expressions are introduced into the original differential equation (24) to obtain

$$-(AD^2_{xhij}u + BD^2_{yhij}u) + CD_{xhij}u + \mathcal{D} D_{yhij}u + ED_x D_{yij}u + GD^2_y D_{xij}u + HD^2_x D_{yij}u + KD^2_x D^2_{yij}u$$
$$= F_{ij} + R_{ij}, \tag{32}$$

where

$$A = \frac{ch}{2}\gamma, \qquad B = \frac{dh}{2}\beta, \tag{33}$$

$$\gamma = \coth\frac{ch}{2a}, \qquad \beta = \coth\frac{dh}{2b}, \tag{34}$$

$$C = c, \qquad \mathcal{D} = d, \tag{35}$$

$$E = \left(\frac{a}{c}\right)^2 \frac{d}{h}\left(\gamma Q - \sinh\frac{ch}{a} + \frac{ch}{a}\right) + \frac{c}{h}\left(\frac{b}{d}\right)^2\left(\beta W - \sinh\frac{dh}{b} + \frac{dh}{b}\right), \tag{36}$$

$$G=-\left(\frac{a}{c}\right)^2\frac{b}{h}\left(\gamma Q-\sinh\frac{ch}{a}+\frac{ch}{a}\right)-\left(\frac{b}{d}\right)^3\frac{c}{h}\left[-\beta W+\sinh\frac{dh}{b}-\frac{1}{3!}\left(\frac{dh}{b}\right)^3-\frac{dh}{b}\right], \tag{37}$$

$$H=-\left(\frac{b}{a}\right)^2\frac{a}{h}\left(\beta W-\sinh\frac{dh}{b}+\frac{dh}{b}\right)-\left(\frac{a}{c}\right)^3\frac{d}{h}\left[-\gamma Q+\sinh\frac{ch}{a}-\frac{1}{3!}\left(\frac{ch}{a}\right)^3-\frac{ch}{a}\right], \tag{38}$$

$$K=-\left(\frac{a}{c}\right)^3\frac{b}{h}\left[\gamma Q-\sinh\frac{ch}{a}-\frac{1}{3!}\left(\frac{ch}{a}\right)^3+\frac{ch}{a}\right]-\left(\frac{b}{d}\right)^3\frac{a}{h}\left[\beta W-\sinh\frac{dh}{b}-\frac{1}{3!}\left(\frac{dh}{b}\right)^3-\frac{dh}{b}\right], \tag{39}$$

$$Q=\cosh\frac{ch}{a}-\frac{1}{2}\left(\frac{ch}{a}\right)^2-1, \qquad W=\cosh\frac{dh}{b}-\frac{1}{2}\left(\frac{dh}{b}\right)^2-1, \tag{40}$$

$$F_{ij}=f_{ij}+ch\coth\left(\frac{ch}{2a}\right)\bar{\bar{F}}^x_{ij}+dh\coth\left(\frac{dh}{2b}\right)\bar{\bar{F}}^y_{ij}-c\bar{F}^x_{ij}-d\bar{F}^y_{ij}, \tag{41}$$

$$R_{ij}=ch\coth\left(\frac{ch}{2a}\right)\bar{\bar{R}}^x_{ij}+dh\coth\left(\frac{dh}{2b}\right)\bar{\bar{R}}^y_{ij}-c\bar{R}^x_{ij}-d\bar{R}^y_{ij}. \tag{42}$$

Expressions for the terms $\bar{\bar{F}}^y_{ij}$, $\bar{F}^y_{ij}$, $\bar{\bar{R}}^y_{ij}$, $\bar{R}^y_{ij}$ and $\bar{R}^x_{ij}$ are defined in Appendix I. If we now return to equation (32) and introduce $O(h^2)$ centred difference approximations for derivatives $D_xD_{yij}u$, $D_x^2D_{yij}u$, $D_y^2D_{xij}u$ and $D_x^2D_y^2u$ (see Appendix I) and neglect R_{ij}, we obtain an $O(h^4)$ nine-point centred difference scheme

$$\begin{aligned}-(AD^2_{xhij}u_h+BD^2_{yhij}u_h)+CD_{xhij}u_h+\mathscr{D}D_{yhij}u_h+ED_{xh}D_{yhij}u_h\\+GD^2_{yh}D_{xhij}u_h+HD^2_{xh}D_{yhij}u_h+KD^2_{xh}D^2_{yhij}u_h=F_{ij}.\end{aligned} \tag{43}$$

The discretization scheme that leads to (43) will herein be referred to as the ONCDS (optimal nine-point centred difference scheme) since it reduces to the optimal (nodally exact) scheme (23) for one-dimensional problems (or when $R_{ij}=0$).

Remarks. This scheme uses a nine-point stencil since a 3×3 matrix of nodes is required to represent all the discrete operators present in (43). The fact that an $O(h^4)$ scheme can be derived for such a compact (3×3) stencil is of significance since it can be applied as close to a boundary as a standard centred difference scheme and still be $O(h^4)$-accurate. Some savings in computational time may be made by using polynomials to approximate the hyperbolic functions present in equations (33)–(42) above.

The optimal tensorial diffusivity follows directly from (43). Setting coefficients $G=H=K=0$, (43) can be written as

$$-\nabla^{\mathrm{T}}_{hij}\cdot(\mathbf{T}\cdot\nabla_{hij}u_h)+\mathbf{V}^{\mathrm{T}}\cdot\nabla_{hij}u_h=F_{ij},$$

where

$$\nabla^{\mathrm{T}}_{hij}=[D_{xhij},D_{yhij}], \qquad \mathbf{V}^{\mathrm{T}}=[C,\mathscr{D}]$$

and the tensorial diffusivity $\mathbf{T}$ is given by

$$\mathbf{T}=\begin{bmatrix}A & E/2\\ E/2 & B\end{bmatrix}.$$

$\mathbf{T}$ is a symmetric tensor which explicitly compensates for truncation errors involving the derivative terms u_{xx}, u_{yy} and u_{xy}. Note that the off-diagonal elements $E/2$ account for the fact that numerical diffusion in any given direction depends not only on the solution gradient in that direction but also on the solution gradients in the perpendicular (crosswind) direction.

Remark. Upon setting $G=H=K=0$ in (43), the difference formulae truncation errors are increased from $O(h^4)$ to $O(h^2)$. It follows that a nodal error estimate of $O(h^2)$ for the approximation $u_h(x_i, y_j)$ may be obtained directly from the method of proof developed by Bramble and Hubbard.[15]

Extension to variable coefficients

In theory, the foregoing analysis can be extended to the case of variable smooth coefficients. Unfortunately, the algebra involved rapidly becomes unwieldy. To simplify the analysis, we limit the representation of high-order terms in the Taylor series expansions of the differential operators, equations (10) and (11), to the leading $O(h^2)$ truncation errors. Such an approach will still yield an $O(h^4)$-accurate scheme. Consider the equation

$$-(au_{xx}+bu_{yy})+cu_x+du_y=f(x, y), \tag{44}$$

where a and b are constants and c, d and f vary spatially. Note that this equation is consistent with the two-dimensional Navier–Stokes equations for constant viscosity. Recall that the expansion (10) for u_x at (x_i, y_j) is

$$D_{xij}u=u_{xij}=D_{hxij}u-\frac{h^2}{3!}D^3_{xij}u+O(h^4). \tag{45}$$

We now wish to represent the $O(h^2)$ term in (45) involving $D^3_{xij}u$ in order to obtain $O(h^4)$ accuracy. Again we use using the differential equation (44). Differentiating (44) once and solving for $D^3_{xij}u$, we obtain

$$D^3_x u=-\frac{b}{a}D^2_y D_x u+\frac{1}{a}D_x c D_x u+\frac{c}{a}D^2_x u+\frac{1}{a}D_x d D_y u+\frac{d}{a}D_y D_x u-\frac{1}{a}D_x f. \tag{46}$$

In order to represent D^3_{xij} in (45) using (46), all differential operators in (46) must be discretized. If we use centred difference operators, which are $O(h^2)$-accurate, on the RHS of (46), we will maintain $O(h^4)$ accuracy overall, since the $D^3_{xij}u$ term in (45) is multiplied by h^2. (It should be noted here that operators other than centred difference could be used for the derivatives in (46), resulting in various schemes with various orders of accuracy.) We obtain

$$\begin{aligned} D_{xij}u=D_{hxij}u-\frac{h^2}{a3!}(cD^2_{hxij}u+D_{hxij}cD_{hxij}u+dD_{hy}D_{hxij}u \\ +D_{hxij}dD_{hyij}u-bD^2_{hy}D_{hxij}u-D_{hxij}f)+O(h^4). \end{aligned} \tag{47}$$

Expressions for $D^2_{xij}u$ (which requires representation of $D^4_x u$), $D_{yij}u$ and $D^2_{yij}u$ are derived in analogous fashion and substituted along with (47) into (44). The result is a nine-point $O(h^4)$ centred difference representation having the same form as equation (43) but with coefficients A, B, etc. given by

$$A=-a+\frac{h^2}{6}\left(D_{hx}c-\frac{c^2}{2a}\right), \tag{48}$$

$$B=-b+\frac{h^2}{6}\left(D_{hy}d-\frac{d^2}{2b}\right), \tag{49}$$

$$C = c + \frac{h^2}{12}\left(D_{hx}^2 c + D_{hy}^2 c - \frac{c}{a} D_{hx} c - \frac{d}{b} D_{hy} c\right), \tag{50}$$

$$\mathscr{D} = d + \frac{h^2}{12}\left(D_{hx}^2 d + D_{hy}^2 d - \frac{c}{a} D_{hx} d - \frac{d}{b} D_{hy} d\right), \tag{51}$$

$$E = \frac{h^2}{12}\left[2(D_{hx} d + D_{hy} c) - cd\left(\frac{1}{a} + \frac{1}{b}\right)\right], \tag{52}$$

$$G = \frac{h^2}{12}\left(\frac{bc}{a} + a\right), \tag{53}$$

$$H = \frac{h^2}{12}\left(\frac{ad}{b} + d\right), \tag{54}$$

$$K = -\frac{h^2}{12}(a + b), \tag{55}$$

$$F = f - \frac{h^2}{12}\left(\frac{c}{a} D_{hx} f + \frac{d}{b} D_{hy} f - D_{hx}^2 f - D_{hy}^2 f\right). \tag{56}$$

We will call this scheme the NCDS (nine-point centred difference scheme) since we have limited the representation of truncation errors in equations (10) and (11) to the leading $O(h^2)$ terms, which can be represented on a 3×3 stencil by using the differential equation and centred difference approximations.

Remarks. A tensorial diffusivity analogous to the one given in the preceding subsection may be derived from (48)–(52). However, note that the coefficients C and $\mathscr{D}$ of the derivatives u_x and u_y must also be modified.

In the present study, derivatives of c and d are approximated with centred difference approximations. Upstream-weighted approximations may be used instead and may prove to be more effective. This issue will be examined in a future study.

NUMERICAL RESULTS

In this section we examine two different test problems. Comparisons are made between analytical and numerically 'exact' solutions and results for the two schemes proposed in this paper, as well as some previously published schemes. The first problem, which has been studied previously by Gupta *et al.*[8] and Stubly *et al.*[11] is a two-dimensional convection–diffusion system with constant convective coefficients. The problem statement is as follows:

$$-(au_{xx} + bu_{yy}) + \alpha\cos(\theta)u_x + \alpha\sin(\theta)u_y = 0 \quad \text{on } (0, 1) \times (0, 1) \tag{57}$$

$$u(x, 0) = u(x, 1) = 0, \qquad 0 \leqslant x \leqslant 1,$$
$$u(0, y) = 4y(1 - y), \qquad u(1, y) = 0, \qquad 0 \leqslant y \leqslant 1. \tag{58}$$

The solution domain for this problem is shown in Figure 4. Equations (57) and (58) describe a steady system which for large α and $\theta = 0$ develops boundary layers along $x = 1$ and $y = 1$. The analytical solution to this problem is given in Appendix II.

The differencing schemes that are included in the comparison are the two proposed higher-order schemes, ONCDS and NCDS, standard first-order upwind differencing (UDS) of the convective terms, centred differencing (CDS), Leonard's[1] upwind differencing scheme (LDS) and

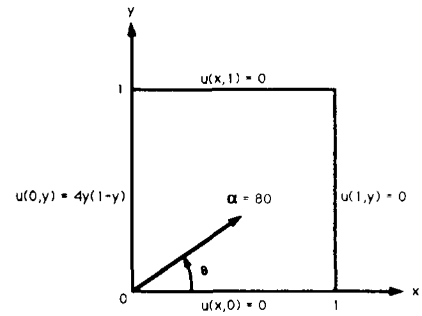

Figure 4. Solution domain showing boundary conditions for the 2D convection–diffusion model problem with constant coefficients (equations (69) and (70))

Table I. Maximum absolute errors at the grid points of the 8 × 8 grid

θ	h^{-1}	UDS	CDS[10]	LDS	QIS[10]	NCDS	ONCDS
0	8	0·0804	0·64	0·2138	0·0046	0·2579	0·0051
	16	0·0245	0·16	0·0141	$0{\cdot}15 \times 10^{-3}$	0.0093	$0{\cdot}2 \times 10^{-4}$
	32	0·0058	$0{\cdot}17 \times 10^{-3}$	$0{\cdot}4 \times 10^{-4}$	$0{\cdot}3 \times 10^{-4}$	$0{\cdot}4 \times 10^{-4}$	$0{\cdot}1 \times 10^{-8}$
$\pi/8$	8	0·3264	0·91	0·2554	0·066	0·2401	0·0335
	16	0·1792	0·12	0·0094	0·0038	0·0082	$0{\cdot}8 \times 10^{-3}$
	32	0·0902	0·0042	0·0015	$0{\cdot}57 \times 10^{-3}$	$0{\cdot}1 \times 10^{-3}$	$0{\cdot}5 \times 10^{-4}$
$\pi/4$	8	0·2721	0·55	0·1708	0·050	0·1931	0·0501
	16	0·1565	0·063	0·0024	0·0024	0·0053	$0{\cdot}9 \times 10^{-3}$
	32	0·0831	0·0047	$0{\cdot}3 \times 10^{-3}$	$0{\cdot}53 \times 10^{-3}$	$0{\cdot}1 \times 10^{-3}$	$0{\cdot}4 \times 10^{-4}$
Order		$O(h)$	$O(h^2)$	$O(h^2)$		$O(h^4)$	$O(h^4)$

the quadratic influence scheme (QIS).[11] Results are computed for $a=b=1$, $\alpha=80$, $\theta=0$, $\pi/8$ and $\pi/4$ and a sequence of uniform meshes $h=1/4$, 1/8, 1/16 and 1/32.

Maximum errors occurring at the grid points of the coarsest grid (8×8, $h=1/8$), are presented in Table I for the various angles θ and grid spacings h. In determining the order of convergence to the exact solution of a particular scheme, it is appropriate to consider the reduction in error at a given point as the grid spacing h is changed. In Table I the reported errors are for a particular point for each scheme and hence show the convergence of that scheme at that point as h changes. As can be seen, the ONCDS scheme is consistently more accurate than the other schemes. Note that the ONCDS and QIS schemes have similar accuracy for $h=1/8$, but since ONCDS exhibits a superior rate of convergence, $O(h^4)$, it is more accurate for the finer grids. QIS and NCDS display similar accuracy on the finer grids tested; however, NCDS will also become more accurate for finer grids because of its $O(h^4)$ rate of convergence. The difference in solution accuracy between LDS and NCDS is marginal for all grids. Again, however, NCDS will exhibit superior accuracy in finer grids since the LDS scheme converges to the exact solution at the suboptimal rate of $O(h^2)$. The $O(h^2)$ CDS scheme, while suitable for the finest grids, is unacceptably inaccurate for the coarser grids. The UDS scheme is also inaccurate, but since it is an $O(h)$ scheme, little improvement is gained with mesh refinement.

Table II provides information similar to that of Table I, except that the maximum errors, wherever they happen to occur on the grid for a given h, are shown. (Convergence rates should not be determined with this table since the error may occur at different points for different values of h.) This table is included in order to demonstrate that the worst errors do not tell a different story than that for Table I. It is still clear that ONCDS is consistently more accurate than any other scheme and that NCDS and LDS display similar accuracy. UDS is as inaccurate as in Table I. Figures 5 and 6 illustrate solution profiles along constant lines $y=0{\cdot}875$ and $x=0{\cdot}25$ respectively for the case $\theta=\pi/4$ and $h=1/8$ for the test problem of equations (57) and (58). It is clear from these figures that ONCDS produces the best results.

For the second test problem the NCDS scheme is extended to the numerical approximation of laminar, viscous, incompressible fluid flow. Consider the two-dimensional Navier–Stokes and

Table II. Maximum absolute grid point errors

θ	h^{-1}	UDS	LDS	NCDS	ONCDS
0	4	0·0408	0·3481	0·3405	0·0213
	8	0·0804	0·2138	0·2579	0·0051
	16	0·1429	0·1192	0·0891	0·0011
$\pi/8$	4	0·2793	0·3332	0·4507	0·1102
	8	0·3264	0·2553	0·2496	0·0335
	16	0·2743	0·1005	0·0737	0·0075
$\pi/4$	4	0·2422	0·3652	0·3206	0·1229
	8	0·2721	0·1708	0·1931	0·0501
	16	0·2677	0·0606	0·0437	0·0144

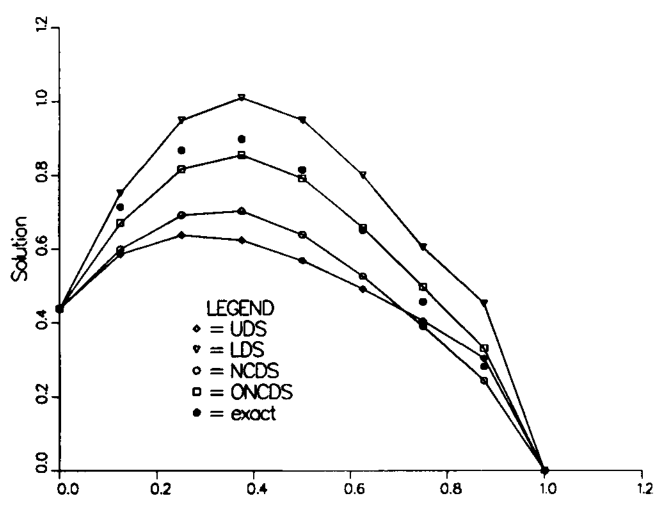

Figure 5. Comparison of results for the two new differencing schemes (ONCDS and NCDS) with results for centred differencing (CDS), upwinding (UDS) and the exact solution for the model problem of Figure 4 for $y=0{\cdot}875$

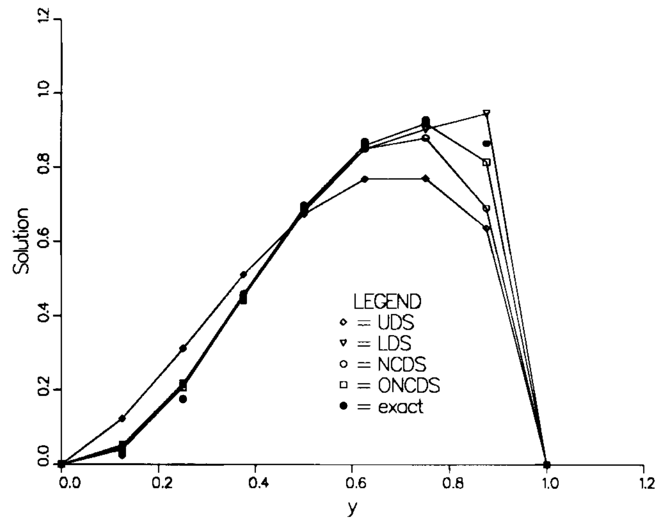

Figure 6. Comparison of results for ONCDS and NCDS with results for CDS, UDS and the exact solution for the model problem of Figure 4 for $x = 0{\cdot}25$

continuity equations

$$\frac{\partial u_j}{\partial t} + u_k \frac{\partial u_j}{\partial x_k} = -\frac{1}{\rho}\frac{\partial p}{\partial x_j} + \nu \frac{\partial^2 u_j}{\partial x_i \partial x_i}, \tag{59}$$

$$\frac{\partial u_k}{\partial x_k} = 0, \tag{60}$$

where $x_k = [x_1, x_2] = [x, y]$, ρ is the density, $u_j = [u, v]$, is the velocity vector, p is the pressure and ν is the kinematic viscosity. If the unsteady and pressure gradient terms in (59) are considered to be source terms, $f(x, y)$, then equations (59) are analogous to the convection–diffusion equation (44). Hence the NCDS discrete equation for (59) has the same form as (43) with coefficients given by (48)–(56), except that the coefficients a and b are constant and equal to ν. While the NCDS scheme has not been applied to the continuity equation for this study, it can and will be applied in future work; standard centred differencing is used for (60).

The problem chosen for study for the application of NCDS to the Navier–Stokes equations is the driven cavity. The domain is a square cavity (1×1) where the top side is moving in a positive direction at constant velocity and the other sides are stationary. The Reynolds number for the flow, based on the velocity of the top side and the width of the cavity, is 400. A uniform grid (30×30) is used.

The NCDS scheme is programmed into an existing semi-implicit code which uses staggered placement of primitive variables and successive overrelaxation while iterating at each time step to achieve a divergence-free velocity field. Since the test problem is steady, the solution is continued until steady state is achieved.

Since the first- and second-derivative operators must be applied to the pressure gradients to provide the necessary terms for the NCDS scheme (see equations (19) and (20) and equations (62) and (63) in Appendix I, as they apply to (43)), it will be required to represent pure and mixed second- and third-order derivatives of pressure. Owing to the staggering of variables, $\partial p/\partial x$ and

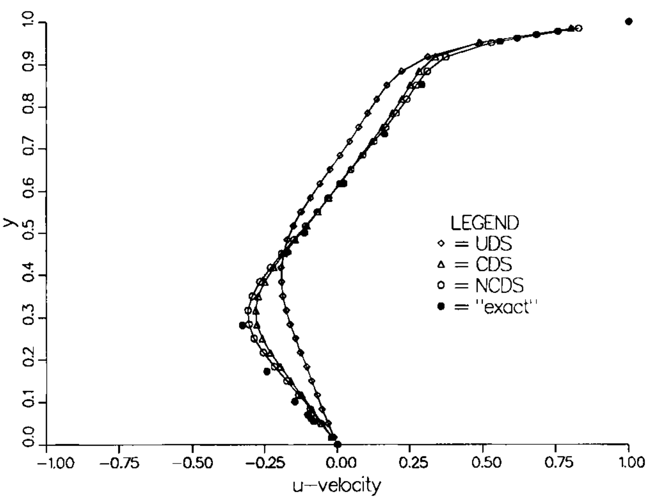

Figure 7. Comparison of results for new scheme (NCDS) with UDS, CDS and the exact numerical solution[14] for a square driven cavity, $Re=400$, for the u-velocity along the constant x-value centreline of the cavity

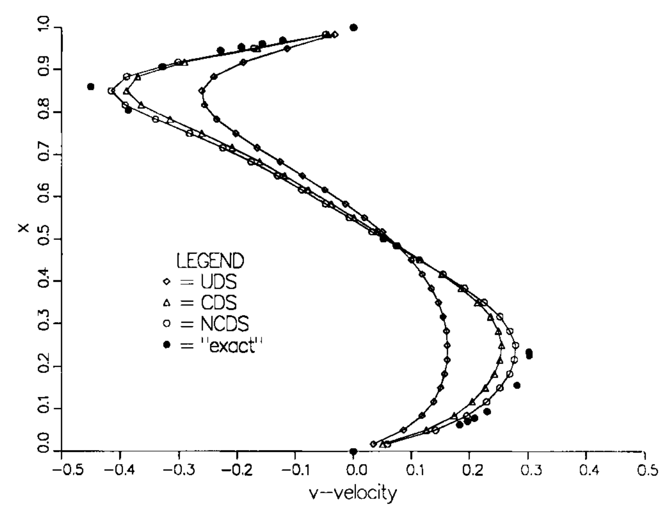

Figure 8. Comparison of results for NCDS with UDS, CDS and the exact numerical solution[14] for a square driven cavity, $Re=400$, for the v-velocity along the constant y-value centreline of the cavity

$\partial p/\partial y$ are easily computed at velocity nodes where they are needed for NCDS. Then, the centred difference operators D_{xhij}, D^2_{xhij}, D_{yhij} and D^2_{yhij} are applied to the pressure gradients computed for the velocity nodes. Discrete time derivatives can also be computed for each velocity node and operated on exactly like the pressure gradients to obtain similarly required mixed derivatives.

Results for the NCDS scheme for the driven cavity test problem are illustrated in Figures 7 and 8 and compared with the UDS and CDS schemes and the 'exact' numerical solution reported by Ghia *et al.*[16] Figure 7 shows results for the u-velocity along the vertical (constant y-value) cavity centreline while Figure 8 shows the v-velocity along the horizontal centreline. The accuracy of the NCDS scheme is clearly superior to that of the other schemes, particularly UDS. The increased accuracy of the NCDS scheme raises the question of the cost effectiveness of employing the $O(h^4)$ scheme with the obvious increased costs of computing the coefficients for the discrete equation. This question is addressed in Appendix III.

Attempts to compute results for higher-Reynolds-number flow ($Re = 1000$) resulted in oscillations for the NCDS scheme. Further development is required to find a more robust but still $O(h^4)$ version of NCDS. Such aspects as determining the optimal type of discrete operators to use for the derivatives that appear in the coefficients (A, B, C and $\mathscr{D}$) in the discrete equation (43) should be pursued. Nevertheless, it has been shown that the ONCDS and NCDS schemes can provide higher-order accuracy than most traditional schemes on a compact stencil.

CONCLUDING REMARKS

In this study we have presented a differential-equation- and Taylor-series-based procedure for obtaining compact high-order difference approximations to elliptic partial differential equations and to transport equations in particular. Using this procedure, we have developed the exact one-dimensional difference scheme, an $O(h^4)$ two-dimensional difference scheme (ONCDS) for constant coefficient convection–diffusion equations and an $O(h^4)$ two-dimensional scheme (NCDS) for convection–diffusion problems with variable convective coefficients. The two-dimensional schemes are derived for a compact 3×3 stencil. While NCDS is equivalent to the schemes proposed in References 8 and 10, the procedure used for its derivation in the present study is simpler and more direct, involving only straightforward differentiation and algebra. The effectiveness of the schemes derived herein has been demonstrated, in terms of accuracy and rates of convergence, for two numerical test problems, including an application of the Navier–Stokes equations.

The approach of representing truncation errors by the governing differential equation has led to a more lucid interpretation of tensorial diffusivity (streamline upwinding) and their relationships to higher-order difference formulae. These relationships will be examined further in future studies. In particular, we plan (i) to investigate various upstream difference approximations to the coefficient and forcing function derivatives present in the higher-order formulae, (ii) to derive an improved high-order scheme and tensorial diffusivity for problems with variable coefficients by considering additional truncation terms and (iii) to extend the methodology to transient problems.

Finally, it is noted that the principle employed in the present study to form high-order difference schemes generalizes to other differential equations provided that appropriate smoothness conditions are satisfied.

ACKNOWLEDGEMENTS

We wish to acknowledge the support of the INEL Long Term Research Initiative in Computational Mechanics and the help of Dr. Graham F. Carey, University of Texas, Austin and Dr. George L. Mesina, INEL for their helpful contributions.

This work was performed under the auspices of the U.S. Dept. of Energy (DOE), Idaho Operations Office, under DOE Contract No. DE-AC07-761D01570, the INEL Long Term Research Initiative in Computational Mechanics.

APPENDIX I: FORMULAE AND CENTRED DIFFERENCE APPROXIMATIONS USED IN THE HIGH-ORDER SCHEMES

This appendix defines the remainder and forcing function expressions for equations (41) and (42) and the $O(h^2)$ centred difference approximations used to represent the cross-derivatives in the $O(h^4)$ formula (43) (see Figure 3 for grid nomenclature).

$$\bar{R}^x_{ij}=\sum_{n=5}^{\infty}\frac{h^{n-1}}{n!}\sum_{k=2}^{n-3}\left(\frac{c}{a}\right)^{n-k-3}D_x^{(k)}\left(\frac{d}{a}D_yD_{xij}u-\frac{b}{a}D_xD^2_{yij}u\right), \tag{61}$$

$$\bar{\bar{F}}^y_{ij}=\sum_{n=1}^{\infty}\frac{h^{2n}}{(2n+2)!}\sum_{k=1}^{2n}\frac{d^{k-1}}{b^k}D_{yij}^{(2n-k+1)}f, \tag{62}$$

$$\bar{F}^y_{ij}=\sum_{n=1}^{\infty}\frac{h^{2n}}{(2n+1)!}\sum_{k=1}^{2n-1}\frac{d^{k-1}}{a^k}D_{yij}^{(2n-k)}f, \tag{63}$$

$$\bar{\bar{R}}^y_{ij}=\sum_{n=6}^{\infty}\frac{h^{n-2}}{n!}\sum_{k=2}^{n-3}\left(\frac{d}{b}\right)^{n-k-3}D_y^{(k)}\left(\frac{c}{b}D_yD_{xij}u-\frac{a}{b}D_yD^2_{xij}u\right), \tag{64}$$

$$\bar{R}^y_{ij}=\sum_{n=5}^{\infty}\frac{h^{n-1}}{n!}\sum_{k=2}^{n-3}\left(\frac{d}{b}\right)^{n-k-3}D_y^{(k)}\left(\frac{c}{b}D_yD_{xij}u-\frac{a}{b}D_yD^2_{xij}u\right), \tag{65}$$

$$D_{xh}D_{yhij}u_h=\frac{1}{4h^2}[u_h(x_{i+1},y_{j+1})-u_h(x_{i-1},y_{j+1})-u_h(x_{i+1},y_{j-1})+u_h(x_{i-1},y_{j-1})], \tag{66}$$

$$\begin{aligned}D_{xh}D^2_{yhij}u_h=\frac{1}{2h^3}[&u_h(x_{i+1},y_{j-1})+u_h(x_{i+1},y_{j+1})+2u_h(x_{i-1},y_j)\\&-u_h(x_{i-1},y_{j+1})-u_h(x_{i-1},y_{j-1})-2u_h(x_{i+1},y_j)],\end{aligned} \tag{67}$$

$$\begin{aligned}D^2_{xh}D_{yhij}u_h=\frac{1}{2h^3}[&u_h(x_{i+1},y_{j+1})+u_h(x_{i-1},y_{j+1})+2u_h(x_i,y_{j-1})\\&-u_h(x_{i-1},y_{j-1})-u_h(x_{i+1},y_{j-1})-2u_h(x_i,y_{j+1})],\end{aligned} \tag{68}$$

$$\begin{aligned}D^2_{xh}D^2_{yhij}u_h=\frac{1}{h^4}[&u_h(x_{i-1},y_{j-1})+u_h(x_{i+1},y_{j-1})+u_h(x_{i+1},y_{j+1})+u_h(x_{i-1},y_{j+1})+4u_h(x_i,y_j)\\&-2u_h(x_i,y_{j+1})-2u_h(x_{i-1},y_j)-2u_h(x_i,y_{j-1})-2u_h(x_{i+1},y_j)].\end{aligned} \tag{69}$$

APPENDIX II: ANALYTICAL SOLUTION TO THE TWO-DIMENSIONAL MODEL PROBLEM

The two-dimensional model problem, restated for convenience, is

$$-(au_{xx}+bu_{yy})+\alpha\cos(\theta)u_x+\alpha\sin(\theta)u_y=0 \quad \text{on } (0,1)\times(0,1), \tag{70}$$

$$\begin{aligned}&u(x,0)=u(x,1)=0, \qquad 0\leqslant x\leqslant 1,\\&u(0,y)=4y(1-y), \qquad u(1,y)=0, \qquad 0\leqslant y\leqslant 1.\end{aligned} \tag{71}$$

The exact solution, also given by Gupta *et al.*,[8] is

$$u(x,y)=\exp\left(-\frac{\alpha}{2}(x\cos\theta+y\sin\theta)\right)\sum_{n=1}^{\infty}\{B_n\sinh[\sigma_n(1-x)]\sin(n\pi y)\}, \tag{72}$$

where

$$\sigma_n^2 = n^2\pi^2 + \alpha^2/4, \tag{73}$$

$$B_n = \frac{8}{\sinh \sigma_n} \int_0^1 y(1-y)\exp\left(\frac{-\alpha y}{2}\sin\theta\right)\sin(n\pi y)\,\mathrm{d}y. \tag{74}$$

APPENDIX III. COST EFFECTIVENESS OF THE $O(h^4)$ SCHEME

It is not possible to give a universally valid assessment of the cost effectiveness of using a higher-order scheme versus a simpler low-order scheme. The difference in employing two different schemes is dependent on the problem being solved, the mesh employed, the method used in the solution algorithm and the programming efficiency of the programer who writes the code. Hence a simple comparison between two schemes has limited validity. Keeping this in mind, we compare the direct costs for constructing the discrete equation and solving it for the $O(h^4)$ NCDS scheme versus an $O(h)$ hybrid upwind/centred difference scheme for the driven cavity problem. We assume that a standard banded Gauss direct solver is used. Table III compares the cost ratio of equation construction and solution of the higher-order scheme with those for the low-order scheme for different mesh widths (neglecting adds). (The width is the side of the mesh which has fewer cells.)

As we can see, the cost of using the $O(h^4)$ scheme is about two times greater than for the $O(h)$ scheme for a mesh of $10\times m$, $m\geqslant 10$. This result indicates, for example, that using the $O(h^4)$ scheme with a 10×10 grid costs the same computationally as the $O(h)$ scheme for a 10×20 grid. However, the rate at which the error decreases for the $O(h^4)$ scheme is eight times faster than for the $O(h)$ scheme since the cell size is halved (assuming we are in the asymptotic error region). That is, the coefficient of the leading truncation term for the $O(h)$ scheme drops by 1/2 as h is halved, while that for the $O(h^4)$ scheme drops by $(1/2)^4 = 1/16$. Clearly, as the mesh is refined, the $O(h^4)$ scheme becomes more cost-effective than the $O(h)$ scheme. It is up to the individual user, however, to determine if his acceptable level of error occurs above or below the cost-effective point.

Table III. Ratio of operations required for construction and solution of NCDS versus a hybrid upwind/centred difference scheme for a driven cavity for various mesh widths

Mesh width (number of cells)	Construction	Solver	Total (construction × solver)
10	1·8	1·21	2·18
20	1·8	1·10	1·98
40	1·8	1·05	1·89
100	1·8	1·02	1·84

REFERENCES

1. B. P. Leonard, 'A stable and accurate convective modelling procedure based on quadratic upstream interpolation', *Comput. Methods Appl. Mech. Eng.*, **19**, 59–98 (1979).
2. M. K. Patel, M. Cross and N. C. Markatos, 'An assessment of flow-oriented schemes for reducing "false diffusion"', *Int. j. numer. methods eng.*, **26**, 2279–2304 (1988).
3. M. A. Leschziner, 'Modeling turbulent recirculating flows by finite-volume methods—current status and future directions', *Int. J. Heat Fluid Flow*, **10**, 186–202 (1989).

4. J. K. Dukowicz and J. D. Ramshaw, 'Tensor viscosity method for convection in numerical fluid dynamics', *J. Comput Phys.*, **32**, 71–79 (1979).
5. T. J. R. Hughes and A. N. Brooks, 'A multidimensional upwind scheme with no crosswind diffusion', in T. J. R. Hughes (ed.), *Finite Element Methods for Convection Dominated Flows, AMD, Vol. 34*, ASME, New York, 1979, pp. 19–35.
6. S. Abarbanel and A. Kumar, 'Compact higher-order schemes for the Euler equations', *J. Sci. Comput.*, **3**, 275–288 (1988).
7. D. J. Jones, J. C. South Jr. and E. B. Klunker, 'On the numerical solution of elliptic partial differential equations by the method of lines', *J. Comput. Phys.*, **9**, 496–527 (1972).
8. M. M. Gupta, R. P. Manohar and J. W. Stephenson, 'A single cell high order scheme for the convection–diffusion equation with variable coefficients', *Int. j. numer. methods fluids*, **4**, 641–651 (1984).
9. S. C. R. Dennis and Q. Wing, 'Generalized finite differences for operators of the Navier–Stokes type,' in D. L. Dwoyer *et al.* (eds), *Proc. 10th Int. Conf. on Numerical Methods in Fluid Dynamics*, Beijing, 1986, *Lecture Notes in Physics, Vol. 264*, Springer, New York, 1987, pp. 222–228.
10. S. C. R. Dennis and J. D. Hudson, 'Compact h^4 finite-difference approximations to operators of Navier–Stokes type', *J. Comput. Phys.*, **85**, 390–416 (1989).
11. G. D. Stubly, G. D. Raithby and A. B. Strong, 'Proposals for a new discrete method based on an assessment of discretization errors', *Numer. Heat Transfer.*, **3**, 411–428 (1980).
12. D. B. Spalding, 'A novel finite difference formulation for differential equations involving both first and second derivatives', *Int. j. numer. methods eng.*, **4**, 551–559 (1972).
13. R. J. MacKinnon and G. F. Carey, 'Analysis of material interface discontinuities and superconvergent fluxes in finite difference theory', *J. Comput. Phys.*, **75**, 151–167 (1988).
14. R. J. MacKinnon and G. F. Carey, 'Superconvergent derivatives: a Taylor series analysis', *Int. j. numer. methods eng.*, **28**, 489–509 (1989).
15. J. H. Bramble and B. E. Hubbard, 'Approximation of derivatives by finite difference methods in elliptic boundary value problems', *Contrib. Diff. Eqns*, **3**, 399–410 (1964).
16. U. Ghia, K. N. Ghia and C. T. Shin, 'High-*Re* solutions for incompressible flow using Navier–Stokes equations and a multigrid method', *J. Comput. Phys.*, **48**, 387–411 (1982).