Received May 1996
Accepted March 1997

Formulation and experiments with high-order compact schemes for nonuniform grids

W.F. Spotz
National Center for Atmospheric Research, Boulder, Colorado, USA and
G.F. Carey
Texas Institute for Computational and Applied Mathematics, ASE-EM Department, University of Texas at Austin, USA

1. Introduction

There is considerable interest in the literature in developing improved local difference schemes (Boisvert, 1981; Leonard, 1979; Leonard and Mokhtari, 1990; Lynch and Rice, 1978; Noye, 1990; Noye and Tan, 1988, 1989). Higher-order schemes that are less compact are also well known (Anderson *et al.*, 1984). Elsewhere, some recent research has focussed on superconvergent properties. The present work concerns a special class of higher-order formulas that are compact. These schemes are nonstandard and operator-specific. They lead to methods that are superconvergent for the class of operators and grids for which they are constructed.

In recent studies we developed a class of high-order compact (HOC) schemes for calculations on uniform grids (MacKinnon and Carey, 1989, 1990) in one and two dimensions. Here the basic approach is to use the differential equation as an additional relation or identity which can be differentiated to eliminate higher-order local truncation errors. For problems with regular coefficients and solutions this strategy yields superconvergent approximations at the grid points. The approach has been applied recently to transport problems (Johnson and MacKinnon, 1992; MacKinnon and Johnson, 1991; Spotz, 1991; Spotz and Carey, 1995, 1996). It is also related to other higher-order schemes (Abarbanel and Kumar, 1988; Boisvert, 1981; Dennis and Hudson, 1989; Dukowicz and Ramshaw, 1979; Gupta and *et al.*, 1982, 1984; Lynch and Rice, 1978; and to the "tau method" (Brandt , 1982) and defect correction approaches (Hemker, 1982).

Most applications of practical interest require some form of mesh grading and the problem of constructing HOC schemes on nonuniform grids has remained open. In the present work we extend the formulation to develop HOC schemes on nonuniform grids in 1D and structured orthogonal graded meshes

This research has been supported in part by grants from the Texas Advanced Technology Program, the UT Enhanced Oil and Gas Recovery Research Project, and the Semiconductor Research Corporation.

in 2D. These two ideas have not previously been combined, and the purpose of this study is to illustrate the complications that result from an HOC scheme on a nonuniform grid.

In the next section we first formulate the HOC scheme for a mapped convection diffusion problem to introduce the main ideas and investigate the algebraic complexity that arises within the compact methodology. We then examine oscillatory behavior and the effect of the associated metric coefficients on rate of convergence in numerical experiments for the model convection diffusion problem. The boundary layer solution is seen to be accurately approximated for a sequence of test problems with increasing Peclet (Reynolds) number. In the final section, we present the HOC formulation for the 2D case using orthogonal graded meshes. The numerical solution for a test problem with exponential layers on two sides is presented to illustrate the method.

2. 1D formulation

As indicated in the introduction, previous work on HOC schemes has been limited to uniform grids. In fact, some of the superconvergence properties associated with these higher-order schemes may be facilitated by cancellation due to the mesh uniformity. However, it should not be inferred that higher order compact schemes cannot be devised for nonuniform grids. Instead, the issue may be one of complexity in deriving such schemes. Here we first introduce one approach for deriving the desired schemes on nonuniform grids in one dimension. Our strategy is motivated by mapping techniques that have been previously utilized for other purposes. This is a natural approach for the present work but we shall also demonstrate that there are some additional considerations that must be addressed both in the 1D and 2D cases.

As a first step, and to clarify the exposition, we restrict the treatment to the 1D case and consider the model convection diffusion equation

$$-\frac{d^2\phi}{dx^2} + u(x)\frac{d\phi}{dx} = s(x), \tag{1}$$

with the familiar boundary conditions $\phi(0) = 0$, $\phi(1) = 1$. When $u \gg 1$ is a constant and $s = 0$ the solution has a steep layer near $x = 1$. The standard 3-point central difference scheme is oscillatory unless the uniform mesh is sufficiently fine. This problem can be alleviated by grading the mesh into the layer. A 3-point scheme on the nonuniform grid can then be easily constructed with truncation error that is reduced to $O(h)$ but error that is statistically $O(h^2)$ (White, 1989). Instead of differencing this way, a mapping strategy may be introduced and a HOC scheme developed as seen below.

Let us construct a map $x = x(\xi)$ to transform (1) from a graded mesh on $0 \leq x \leq 1$ to a uniform mesh on $0 \leq \xi \leq 1$. The transformed equation is simply

$$-\left(\frac{d\xi}{dx}\right)^2 \frac{d^2\hat{\phi}}{d\xi^2} + \left(\hat{u}\frac{d\xi}{dx} - \frac{d^2\xi}{dx^2}\right)\frac{d\hat{\phi}}{d\xi} = \hat{s}, \tag{2}$$

where $\hat{\phi}(\xi) = \phi(x)(\xi))$, $\hat{u}(\xi) = u(x(\xi))$, $\hat{s}(\xi) = s(x(\xi))$, and the metric coefficients $\frac{d\xi}{dx}$ and $\frac{d^2\xi}{dx^2}$ now enter the formulation.

Provided the map is regular and non-degenerate (so that $\frac{d\xi}{dx} \neq 0$) we can write (2) conveniently in the form

$$-\frac{d^2\hat{\phi}}{d\xi^2} + c(\xi)\frac{d\hat{\phi}}{d\xi} = f(\xi), \tag{3}$$

where

$$\overline{c(\xi)} \equiv \frac{\hat{u}\frac{d\xi}{dx} - \frac{d^2\xi}{dx^2}}{\left(\frac{d\xi}{dx}\right)^2}, \quad f(\xi) \equiv \frac{\hat{s}}{\left(\frac{d\xi}{dx}\right)^2}. \tag{4}$$

Next, we construct a HOC scheme for the transformed variable coefficient problem in (3). Central differencing (3) on a uniform grid (ξ_i) of mesh size h we obtain

$$-\delta_\xi^2\hat{\phi}_i + c_i\delta_\xi\hat{\phi}_i - \tau_i = f_i, \tag{5}$$

where $\hat{\phi}_i = \hat{\phi}(\xi_i)$, $c_i = c(\xi_i)$, etc., and δ_ξ, δ_ξ^2 denote the standard 3-point $O(h^2)$ central difference operators for the first and second derivatives with respect to ξ. The local truncation error τ_i in (5) has the form

$$\tau_i = \frac{h^2}{12}\left[2c\frac{d^3\hat{\phi}}{d\xi^3} - \frac{d^4\hat{\phi}}{d\xi^4}\right]_i + O(h^4), \tag{6}$$

where the subscript indicates evaluation at grid point i.

A fourth-order formulation may be constructed by appropriately differentiating (3) to obtain a suitable representation for the leading truncation error terms in (6) and then differencing this representation accordingly. For example, from (3)

$$\begin{aligned}\left.\frac{d^3\hat{\phi}}{d\xi^3}\right|_i &= \left[c\frac{d^2\hat{\phi}}{d\xi^2} + \frac{dc}{d\xi}\frac{d\hat{\phi}}{d\xi} - \frac{df}{d\xi}\right]_i, \\ &= [c_i\delta_\xi^2 + \delta_\xi c_i\delta_\xi]\hat{\phi}_i - \delta_\xi f_i + O(h^2).\end{aligned}$$

A similar relation can be derived for $\left.\frac{d^4\phi}{d\xi^4}\right|_i$.

Substituting these expressions into (6) and incorporating the results in (5) yields the HOC scheme for the mapped problem:

$$-A_i\delta_\xi^2\hat{\phi}_i + C_i\delta_\xi\hat{\phi}_i = f_i - \frac{h^2}{12}\left[-\delta_\xi^2 + c_i\delta_\xi\right] f_i + O(h^4), \tag{7}$$

where

$$A_i = 1 + \frac{h^2}{12}\left(c_i^2 - 2\delta_\xi c_i\right), \quad C_i = c_i + \frac{h^2}{12}\left(\delta_\xi^2 c_i - c_i\delta_\xi c_i\right), \tag{8}$$

with c_i and f_i defined by (4). Formally, this provides a compact 3-point scheme that promises to be superconvergent with $O(h^4)$ accuracy at the nodes of the nonuniform grid. However, note that the coefficients in (8) involve differences of the rational expressions in (4) and these, in turn, contain first and second derivatives of the transformation function. This implies not only more computational work to implement (7), but also raises some important open questions concerning the effect of the transformation and difference approximations in the compact formulation. In the next sections we construct three numerical experiments to illustrate this point. In the first experiment, $x(\xi)$ is given as a smooth function. Next the map is not specified analytically and the derivatives in (4) are differenced. Numerical tests to investigate rates of convergence and also the accuracy of layer approximation with increasing convection are included. These results then motivate a strategy in Section 4 on high-order metrics, and the extension in Section 5 to two dimensions.

3. 1D experiments

Consider the test problem (1) with u = constant, $s = 0$. The analytic solution is $\phi(x) = (e^{ux} - 1)/(e^u - 1)$ and for $u \gg 1$ has a steep layer near $x = 1$. To illustrate the idea let us introduce the mapping function

$$x(\xi) = \xi + \frac{\gamma}{\pi}\sin \pi\xi, \quad 0 \le \xi \le 1, \tag{9}$$

where γ is the grading parameter. The map is invertible for $|\gamma| < 1$; $\gamma > 0$ corresponds to compression (clustering) to the right and similarly to the left for $\gamma < 0$. In the following calculations we choose $\gamma = ½$ which corresponds to a moderate grading to the right.

The test problem was computed on a sequence of uniformly refined grids $h = \frac{1}{4}, \frac{1}{8}, \ldots \frac{1}{64}$ for $u = 5$ and $u = 20$. The error $E = |\phi(x_i) - \phi_i|$ at representative grid point $x_i = x(\xi_i = 0.75)$ is graphed in Figure 1 against mesh size h on a log-log scale for the central difference scheme (CDS), upwind difference scheme (UDS) and high-order compact (HOC) scheme. The rate exponent m is given by the asymptotic slope of the curves. The calculations for the high-order scheme utilize full knowledge of the analytic map (9) to compute the metric derivatives $\frac{d\xi}{dx}$ and $\frac{d^2\xi}{dx^2}$ exactly, and the optimal superconvergent $O(h^4)$ rate at x_i is obtained.

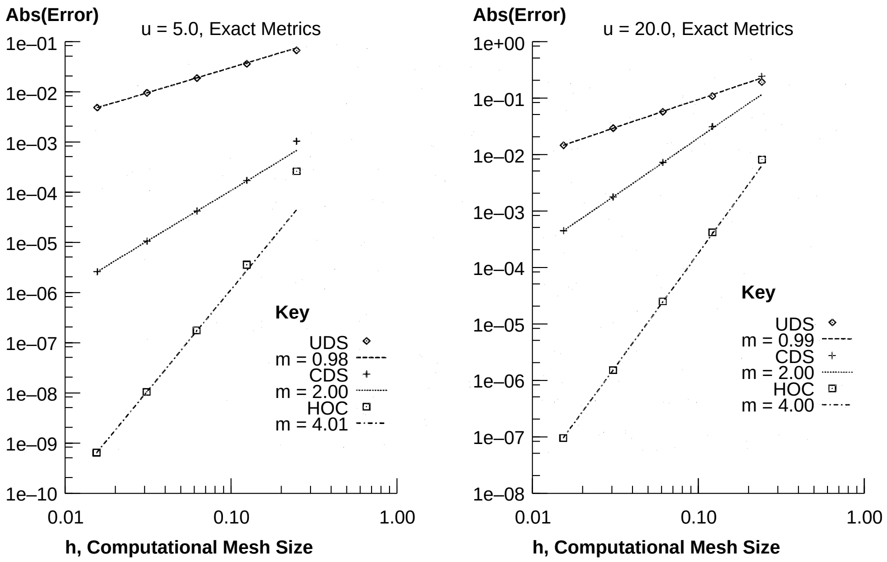

Figure 1.
Convergence results for 1D convection diffusion on a nonuniform grid with exact metrics, u = 5 and 20

In practice, the map may not be specified analytically and the metric coefficients may have to be differenced. We examine the effect of this approximation using the grid from the preceding test. That is, we take precisely the nonuniform grid generated by (9) and evaluate the entries in (4) at each point by locally differencing for $\frac{d\xi}{dx}$ and $\frac{d^2\xi}{dx^2}$ This would be a natural approach given an arbitrary graded mesh (x_i). The results for the compact formula (7) with this approximation are summarized in Figure 2. Note that the effect of approximating the metric derivatives by differences is to degrade the asymptotic rate of the HOC scheme reducing it to $O(h^2)$. The approximate solution for the central and higher-order schemes are essentially identical for u = 5. However, there is a redeeming feature: when the convection is increased to u = 20 the higher order scheme is almost an order of magnitude more accurate. Furthermore, comparisons of the two solutions for greater convection (u = 50) on a coarse nonuniform grid of eight cells generated by (9) reveals that the HOC scheme is nonoscillatory whereas the CDS still produces an oscillatory result (Figure 3). This nonoscillatory property for the HOC scheme has been theoretically proven in 1D for uniform grids (MacKinnon and Johnson, 1991; Spotz, 1991).

The HOC results in Figure 3 are encouraging but the mesh gradation is mild and the Peclet number of 50 is quite moderate so the boundary layer near x = 1 is relatively modest. The ability of the method to function with more strongly graded meshes and at higher convection levels is therefore relevant. In fact, if faithful representation of the layer structure is desired then the mesh should be graded so that there are a few grid points within the layer. Consequently, we considered the test problem for successively increasing convection levels

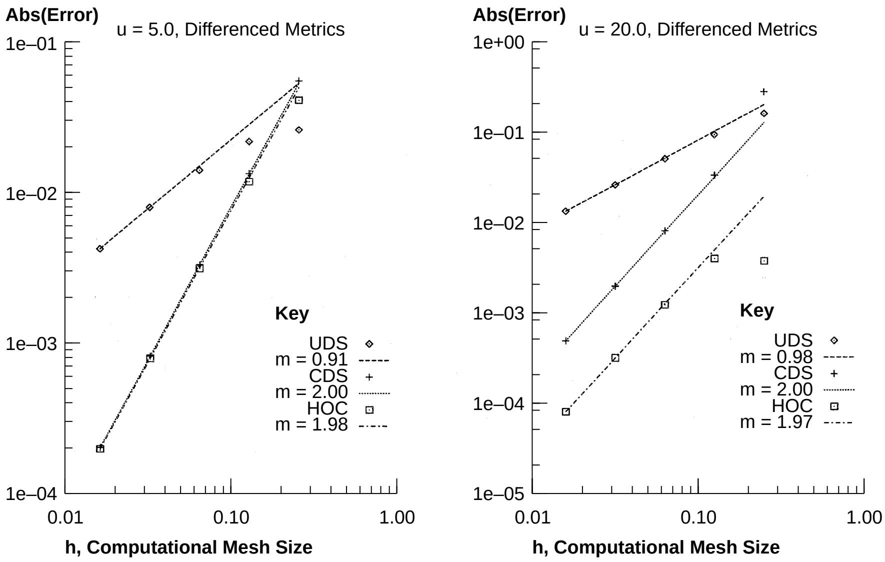

Figure 2. Convergence results for 1D convection diffusion on a nonuniform grid with differenced metrics, u = 5 and 20

corresponding to u = 50, 100, 250, and 500. The same grading function (9) was applied with γ =0.6, 0.7, 0.8, and 0.9 respectively. It can be shown for this problem that the boundary layer thickness, defined at the point where ϕ = 0.01, is approximately 4.6/u when $u \gg 5$. This result was used to choose a unique h in each of the four cases such that three cells lie within the boundary layer. The HOC results in the layer regions are graphed in Figure 4 and compared with the

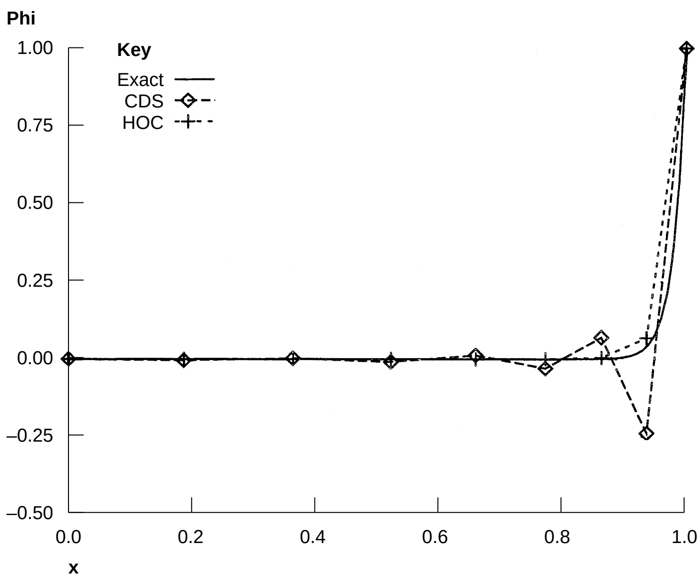

Figure 3. 1D convection diffusion results for the exact, oscillating CDS, and HOC scheme with differenced metrics, u = 50, h = ⅛, on a nonuniform grid

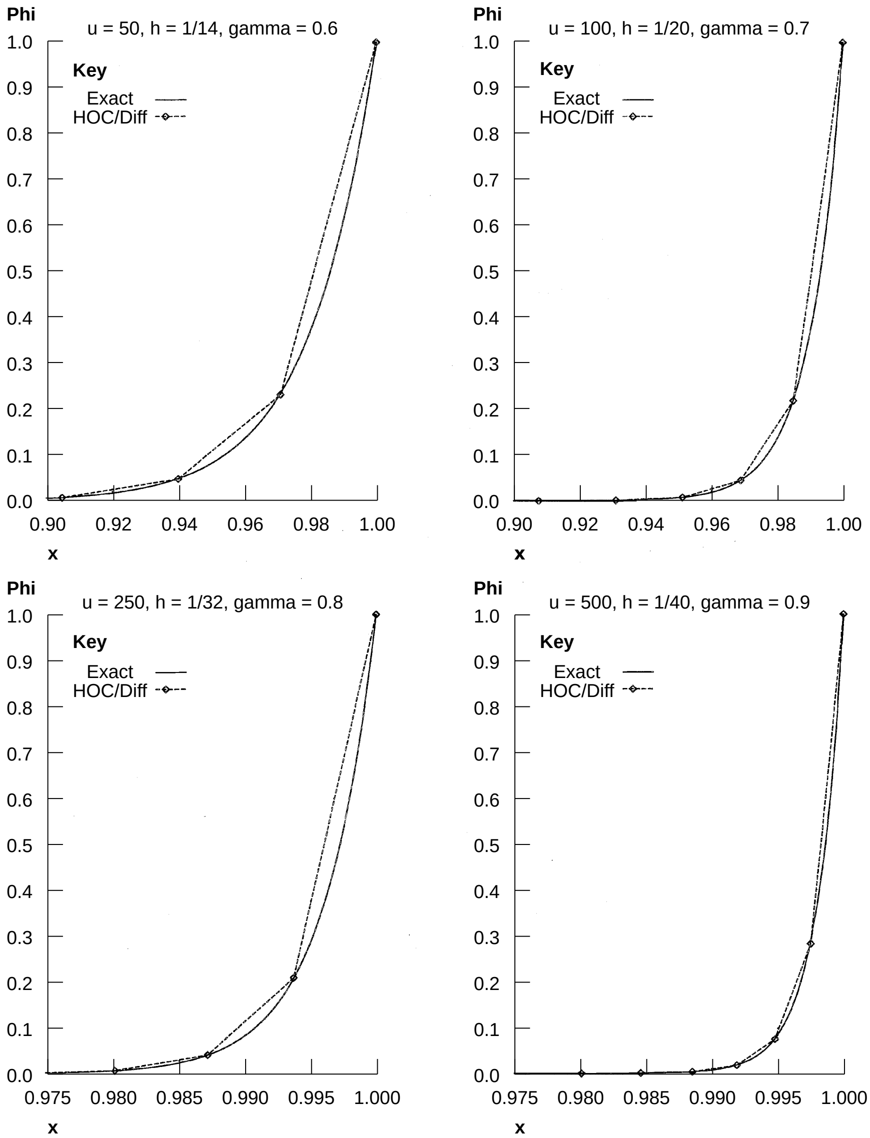

Figure 4.
Boundary layer results for HOC scheme with differenced metrics

analytical solution. The nodal superconvergence property is evident in each case and the approximation of the layer is indeed excellent.

4. High-order compact metrics

If the map $x(\xi)$ is not known explicitly, it may have been generated by the numerical solution of some differential equation (as in PDE grid generators). It is then possible to recover the full $O(h^4)$ estimate suggested by (7) in a manner analogous to the way in which the HOC scheme was developed for the governing transport equation. To illustrate this idea, let us introduce the boundary value problem

$$\frac{d^2x}{d\xi^2} + \pi^2 x = \pi^2 \xi, \tag{10}$$

with boundary conditions $x(0)$ 0, $x(1) = 1$, which corresponds to a Helmholtz PDE grid generator in 1D with a positive source term proportional to ξ. The exact solution is precisely the grading function $x(\xi)$ in (9). Let us assume now that the grid (and indirectly the map) is generated by solving (10) accurately using a uniform grid. Now (10) can be used as an auxiliary relation for the difference approximation of the metrics $\frac{d\xi}{dx}$ and $\frac{d^2\xi}{dx^2}$ at grid point i. More specifically, $\frac{d\xi}{dx} = \frac{1}{dx/d\xi}$, so

$$\left.\frac{d\xi}{dx}\right|_i = \frac{1}{\delta_\xi x_i - \frac{h^2}{6}\left.\frac{d^3x}{d\xi^3}\right|_i + O(h^4)}.$$

Using (10),

$$\begin{aligned}\left.\frac{d\xi}{dx}\right|_i &= \frac{1}{\delta_\xi x_i - \frac{h^2\pi^2}{6}\left(1 - \frac{dx}{d\xi}\right)_i + O(h^4)}, \\ &= \frac{1}{\left(1 + \frac{h^2\pi^2}{6}\right)\delta_\xi x_i - \frac{h^2\pi^2}{6}} + O(h^4),\end{aligned} \tag{11}$$

where we have used the identity $\frac{1}{1+\varepsilon} = 1 - \varepsilon + \varepsilon_2 - \ldots$ to determine the order of magnitude of the truncation error. Similarly, since $d^2\xi/dx^2 = (-d^2x/dx^2)/((dx/d\xi)^3)$, we can use (11) to obtain an $O(h^4)$ approximation to $\frac{d^2\xi}{dx^2}$:

$$\left.\frac{d^2\xi}{dx^2}\right|_i = \frac{-\pi^2(\xi_i - x_i)}{\left[\left(1 + \frac{h^2\pi^2}{6}\right)\delta_\xi x_i - \frac{h^2\pi^2}{6}\right]^3} + O(h^4). \tag{12}$$

Before equations (11) and (12) can be used in (4) to recover the optimal $O(h^4)$ result, we must consider the endpoints. Equations (7) and (8) require that the function c must be differenced in order to apply the HOC scheme on an interior point. The definition of c in (4) thus necessitates an approximation of the grid metrics at the endpoints. Fortunately, the form of (8) requires only $O(h^2)$ accuracy for these terms in order to maintain an overall $O(h^4)$ method.

Letting δ_ξ^+ represent the forward difference operator,

$$\left.\frac{d\xi}{dx}\right|_i = \frac{1}{\delta_\xi^+ x_i - \frac{h}{2}\left.\frac{d^2x}{d\xi^2}\right|_i + O(h^2)}.$$

Using (10) again,

$$\left.\frac{d\xi}{dx}\right|_i = \frac{1}{\delta_\xi^+ x_i - \frac{h}{2}\pi^2(\xi_i - x_i)} + O(h^2).$$

At the left endpoint, $i = 1$, and $x_1 = \xi_1 = 0$, so

$$\left.\frac{d\xi}{dx}\right|_1 = \frac{1}{\delta_\xi^+ x_1} + O(h^2),$$

and $\frac{d^2\xi}{dx^2}$ can be computed from (12). The right endpoint is treated similarly:

$$\left.\frac{d\xi}{dx}\right|_N = \frac{1}{\delta_\xi^- x_N} + O(h^2),$$

where N is the rightmost grid point and δ_ξ^- represents the backward difference operator for the first derivative with respect to ξ.

Figure 5 shows the convergence results for the case where the metrics are computed using this auxiliary equation. The HOC method does in fact recover the optimal $O(h^4)$ result.

Remark. As an alternative to utilizing a relation such as (10) in this way, one could simply use more adjacent grid points to approximate the metric derivatives more accurately. While this is counter to the goals of a compact representation, it may be acceptable since the grid metric coefficients can be computed explicitly prior to constructing the HOC stencils. For example, the

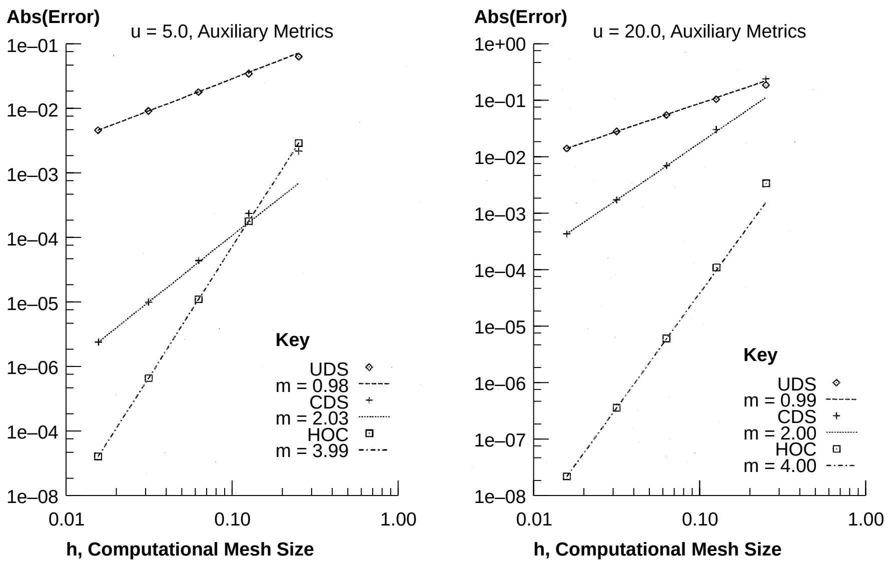

Figure 5.
Convergence results for 1D convection diffusion on a nonuniform grid with approximated metrics using an auxiliary equation, u = 5 and 20

mapping $x(\zeta)$ could be constructed for a set of points $\{x_i\}$ using the Lagrange basis on the domain.

Another approach would be to generate an approximate grid mapping function as Ribbens (1989) does. This smooths the grid in a least-squares sense and ensures that the high-order derivatives exist, as required by the HOC scheme. The implication is that the HOC scheme (7) can be constructed even for very irregular grids in 1D where there is no specified algebraic mapping function or PDE grid generator a priori.

5. 2D formulation

This section extends the approach of Section 2 from 1D to 2D. Accordingly, we begin with 2D convection diffusion on the physical domain Ω,

$$-\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}\right)+u(x,y)\frac{\partial\phi}{\partial x}+v(x,y)\frac{\partial\phi}{\partial y}=f(x,y), \tag{13}$$

where u and v are variable convection coefficients and f is the forcing function. We now transform the equation to a computational domain $\hat{\Omega}$ via mapping functions $x = x(\xi, \eta)$ and $y = y(\xi, \eta)$. If we let $\hat{\phi}(\xi, \eta) = \phi(x(\xi, \eta), y(\xi, \eta))$, etc. the transformed equation is

$$\begin{aligned}a(\xi,\eta)\frac{\partial^2\hat{\phi}}{\partial\xi^2}+g(\xi,\eta)\frac{\partial^2\hat{\phi}}{\partial\xi\partial\eta}+b(\xi,\eta)\frac{\partial^2\hat{\phi}}{\partial\eta^2}+&\\ c(\xi,\eta)\frac{\partial\hat{\phi}}{\partial\xi}+d(\xi,\eta)\frac{\partial\hat{\phi}}{\partial\eta} &= \hat{f}(\xi,\eta),\end{aligned} \tag{14}$$

where

$$a(\xi,\eta)=-\left(\frac{\partial\xi}{\partial x}\right)^2-\left(\frac{\partial\xi}{\partial y}\right)^2,\qquad b(\xi,\eta)=-\left(\frac{\partial\eta}{\partial x}\right)^2-\left(\frac{\partial\eta}{\partial y}\right)^2,$$

$$c(\xi,\eta)=\hat{u}\frac{\partial\xi}{\partial x}+\hat{v}\frac{\partial\xi}{\partial y}-\frac{\partial^2\xi}{\partial x^2}-\frac{\partial^2\xi}{\partial y^2},\qquad d(\xi,\eta)=\hat{u}\frac{\partial\eta}{\partial x}+\hat{v}\frac{\partial\eta}{\partial y}-\frac{\partial^2\eta}{\partial x^2}-\frac{\partial^2\eta}{\partial y^2},$$

$$g(\xi,\eta)=-2\left(\frac{\partial\xi}{\partial x}\frac{\partial\eta}{\partial x}+\frac{\partial\xi}{\partial y}\frac{\partial\eta}{\partial y}\right).$$

There are two significant complications to (14) which do not occur in the 1D case (3).

First, there is now a second-order cross derivative present in the governing equation, which heretofore has not been approximated in a HOC formulation. Second, there are three second-order derivatives to model, each with an independent and variable coefficient, preventing us from scaling the problem to yield a diffusion coefficient of unity. Thus we require a new HOC formulation which is much more algebraically complicated than those previously derived.

We begin, as always, by applying central differencing to (14) at node ij, which gives

$$a_{ij}\delta_\xi^2\hat{\phi}_{ij} + g_{ij}\delta_\xi\delta_\eta\hat{\phi}_{ij} + b_{ij}\delta_\eta^2\hat{\phi}_{ij} + c_{ij}\delta_\xi\hat{\phi}_{ij} + d_{ij}\delta_\eta\hat{\phi}_{ij} - \tau_{ij} = \hat{f}_{ij}, \tag{15}$$

where the truncation error, τ_{ij} is given by

$$\tau_{ij} = \frac{h^2}{12}\left[a\frac{\partial^4\hat{\phi}}{\partial\xi^4} + 2g\left(\frac{\partial^4\hat{\phi}}{\partial\xi^3\partial\eta} + \frac{\partial^4\hat{\phi}}{\partial\xi\partial\eta^3}\right) + b\frac{\partial^4\hat{\phi}}{\partial\eta^4} + 2c\frac{\partial^3\hat{\phi}}{\partial\xi^3} + 2d\frac{\partial^3\hat{\phi}}{\partial\eta^3}\right]_{ij} + O(h^4). \tag{16}$$

Note that there are six (6) derivatives in the h^2-term of the truncation error. Our HOC theory seeks to find alternative representations for these derivatives by differentiating the governing equation (14). Let us begin by differentiating (14) with respect to ξ and rearrange to get

$$\frac{\partial^3\hat{\phi}}{\partial\xi^3} = \frac{1}{a}\left[\frac{\partial\hat{f}}{\partial\xi} - \left(\frac{\partial a}{\partial\xi} + c\right)\frac{\partial^2\hat{\phi}}{\partial\xi^2} - \left(\frac{\partial g}{\partial\xi} + d\right)\frac{\partial^2\hat{\phi}}{\partial\xi\partial\eta} - g\frac{\partial^3\hat{\phi}}{\partial\xi^2\partial\eta} - \frac{\partial b}{\partial\xi}\frac{\partial^2\hat{\phi}}{\partial\eta^2} - b\frac{\partial^3\hat{\phi}}{\partial\xi\partial\eta^2} - \frac{\partial c}{\partial\xi}\frac{\partial\hat{\phi}}{\partial\xi} - \frac{\partial d}{\partial\xi}\frac{\partial\hat{\phi}}{\partial\eta}\right]. \tag{17}$$

Similarly, with respect to η,

$$\frac{\partial^3\hat{\phi}}{\partial\eta^3} = \frac{1}{b}\left[\frac{\partial\hat{f}}{\partial\eta} - \left(\frac{\partial b}{\partial\eta} + d\right)\frac{\partial^2\hat{\phi}}{\partial\eta^2} - \left(\frac{\partial g}{\partial\eta} + c\right)\frac{\partial^2\hat{\phi}}{\partial\xi\partial\eta} - g\frac{\partial^3\hat{\phi}}{\partial\xi\partial\eta^2} - \frac{\partial a}{\partial\eta}\frac{\partial^2\hat{\phi}}{\partial\xi^2} - a\frac{\partial^3\hat{\phi}}{\partial\xi^2\partial\eta} - \frac{\partial c}{\partial\eta}\frac{\partial\hat{\phi}}{\partial\xi} - \frac{\partial d}{\partial\eta}\frac{\partial\hat{\phi}}{\partial\eta}\right]. \tag{18}$$

Expressions for $\frac{\partial^4\hat{\phi}}{\partial\xi^4}$ and $\frac{\partial^4\hat{\phi}}{\partial\eta^4}$ are found by differentiating twice and rearranging:

$$a\frac{\partial^4\hat{\phi}}{\partial\xi^4} = \frac{\partial^2\hat{f}}{\partial\xi^2} - \left(\frac{\partial^2 a}{\partial\xi^2} + 2\frac{\partial c}{\partial\xi}\right)\frac{\partial^2\hat{\phi}}{\partial\xi^2} - \left(2\frac{\partial a}{\partial\xi} + c\right)\frac{\partial^3\hat{\phi}}{\partial\xi^3} - \left(\frac{\partial^2 g}{\partial\xi^2} + 2\frac{\partial d}{\partial\xi}\right)\frac{\partial^2\hat{\phi}}{\partial\xi\partial\eta} - \left(2\frac{\partial g}{\partial\xi} + d\right)\frac{\partial^3\hat{\phi}}{\partial\xi^2\partial\eta} - g\frac{\partial^4\hat{\phi}}{\partial\xi^3\partial\eta} - \frac{\partial^2 b}{\partial\xi^2}\frac{\partial^2\hat{\phi}}{\partial\eta^2} - 2\frac{\partial b}{\partial\xi}\frac{\partial^3\hat{\phi}}{\partial\xi\partial\eta^2} - b\frac{\partial^4\hat{\phi}}{\partial\xi^2\partial\eta^2} - \frac{\partial^2 c}{\partial\xi^2}\frac{\partial\hat{\phi}}{\partial\xi} - \frac{\partial^2 d}{\partial\xi^2}\frac{\partial\hat{\phi}}{\partial\eta}, \tag{19}$$

$$\begin{aligned} b\frac{\partial^4\hat{\phi}}{\partial\eta^4} = & \frac{\partial^2\hat{f}}{\partial\eta^2} - \left(\frac{\partial^2 b}{\partial\eta^2} + 2\frac{\partial d}{\partial\eta}\right)\frac{\partial^2\hat{\phi}}{\partial\eta^2} - \left(2\frac{\partial b}{\partial\eta} + d\right)\frac{\partial^3\hat{\phi}}{\partial\eta^3} - \\ & \left(\frac{\partial^2 g}{\partial\eta^2} + 2\frac{\partial c}{\partial\eta}\right)\frac{\partial^2\hat{\phi}}{\partial\xi\partial\eta} - \left(2\frac{\partial g}{\partial\eta} + c\right)\frac{\partial^3\hat{\phi}}{\partial\xi\partial\eta^2} - g\frac{\partial^4\hat{\phi}}{\partial\xi\partial\eta^3} - \\ & \frac{\partial^2 a}{\partial\eta^2}\frac{\partial^2\hat{\phi}}{\partial\xi^2} - 2\frac{\partial a}{\partial\eta}\frac{\partial^3\hat{\phi}}{\partial\xi^2\partial\eta} - a\frac{\partial^4\hat{\phi}}{\partial\xi^2\partial\eta^2} - \frac{\partial^2 c}{\partial\eta^2}\frac{\partial\hat{\phi}}{\partial\xi} - \frac{\partial^2 d}{\partial\eta^2}\frac{\partial\hat{\phi}}{\partial\eta}. \end{aligned} \quad (20)$$

Equations (17-20) provide us with independent substitutions for four of the six derivatives in (16), leaving $\partial^4\phi/\partial\xi^3\partial\eta$ and $\partial^4\phi/\partial\xi^\partial\eta^3$ unaccounted for. Unfortunately, there is only the potential for one more auxiliary equation (obtained by differentiating (14) by both ξ and η), which is not sufficient to provide compact representations for both of these derivatives, unless some further restriction is placed on the governing equation.

Note, however, that both these derivatives are scaled by g in (16), and that $g = 0$ is identically true for orthogonal grids. Imposing this restriction, the resulting HOC formula is

$$\begin{aligned} & A_{ij}\delta_\xi^2\hat{\phi}_{ij} + G_{ij}\delta_\xi\delta_\eta\hat{\phi}_{ij} + B_{ij}\delta_\eta^2\hat{\phi}_{ij} + C_{ij}\delta_\xi\hat{\phi}_{ij} + D_{ij}\delta_\eta\hat{\phi}_{ij} + \\ & \frac{h^2}{12}\Big[(a_{ij} + b_{ij})\,\delta_\xi^2\delta_\eta^2\hat{\phi}_{ij} + (2\delta_\eta a_{ij} + d_{ij} + \beta_{ij}a_{ij})\delta_\xi^2\delta_\eta\hat{\phi}_{ij} + \\ & \quad (2\delta_\xi b_{ij} + c_{ij} + \alpha_{ij}b_{ij})\delta_\xi\delta_\eta^2\hat{\phi}_{ij}\Big] = F_{ij} + O(h^4), \end{aligned} \quad (21)$$

where the coefficients are given by

$$\begin{aligned} A_{ij} = & \; a_{ij} + \frac{h^2}{12}\left[\delta_\xi^2 a_{ij} + \delta_\eta^2 a_{ij} + 2\delta_\xi c_{ij} + \alpha_{ij}(\delta_\xi a_{ij} + c_{ij}) + \right. \\ & \left. \beta_{ij}\delta_\eta a_{ij}\right], \end{aligned} \quad (22)$$

$$\begin{aligned} B_{ij} = & \; b_{ij} + \frac{h^2}{12}\left[\delta_\xi^2 b_{ij} + \delta_\eta^2 b_{ij} + 2\delta_\eta d_{ij} + \beta_{ij}(\delta_\eta b_{ij} + d_{ij}) + \right. \\ & \left. \alpha_{ij}\delta_\xi b_{ij}\right], \end{aligned} \quad (23)$$

$$C_{ij} = c_{ij} + \frac{h^2}{12}\left[\delta_\xi^2 c_{ij} + \delta_\eta^2 c_{ij} + \alpha_{ij}\delta_\xi c_{ij} + \beta_{ij}\delta_\eta c_{ij}\right], \quad (24)$$

$$D_{ij} = d_{ij} + \frac{h^2}{12}\left[\delta_\xi^2 d_{ij} + \delta_\eta^2 d_{ij} + \alpha_{ij}\delta_\xi d_{ij} + \beta_{ij}\delta_\eta d_{ij}\right], \quad (25)$$

$$F_{ij} = \hat{f}_{ij} + \frac{h^2}{12}\left[\delta_\xi^2 \hat{f}_{ij} + \delta_\eta^2 \hat{f}_{ij} + \alpha_{ij}\delta_\xi \hat{f}_{ij} + \beta_{ij}\delta_\eta \hat{f}_{ij}\right], \quad (26)$$

$$G_{ij} = \frac{h^2}{12}\left[2\delta_\eta c_{ij} + 2\delta_\xi d_{ij} + \alpha_{ij}d_{ij} + \beta_{ij}c_{ij}\right], \quad (27)$$

with α_{ij} and β_{ij} given by

$$\alpha_{ij} = \frac{c_{ij} - 2\delta_\xi a_{ij}}{a_{ij}},$$
$$\beta_{ij} = \frac{d_{ij} - 2\delta_\eta b_{ij}}{b_{ij}}.$$

To illustrate the 2D nonuniform HOC treatment we consider a 2D convection diffusion test case with solution $\phi = (1 - l(x))(1 - l(y))$ where $l(x)$ denotes the layer function in the 1D case considered previously. Dirichlet data corresponding to this solution are specified on each edge of the unit square and the convection velocity vector has magnitude 50 at a 45° angle above the x-axis. By inspection, the solution is close to unity over most of the domain with boundary layers adjacent to sides $x = 1$ and $y = 1$ where the solution decays rapidly to satisfy the boundary condition $\phi = 0$.

Since the test problem has layer behavior on two sides, a nonuniform graded mesh into each layer zone is very appropriate. Accordingly, we take the previous grading function (9) in each direction. This generates a tensor product orthogonal grid that is progressively graded into the two wall layers. As a representative numerical test we set $\gamma = 0.6$ in (9) in each direction and solved the problem with the stated velocity vector using 15 grid points in each direction. The solution surface and contours obtained with this HOC scheme are shown in Figure 6 and are visually indistinguishable from the exact solution. Figure 7 shows the convergence results for UDS, CDS, and HOC for this 2D model problem with convection $Re = 50$ and 100 at a grading factor $\gamma = 0.5$. The exact grid mapping is utilized, and the expected rates of convergence are observed.

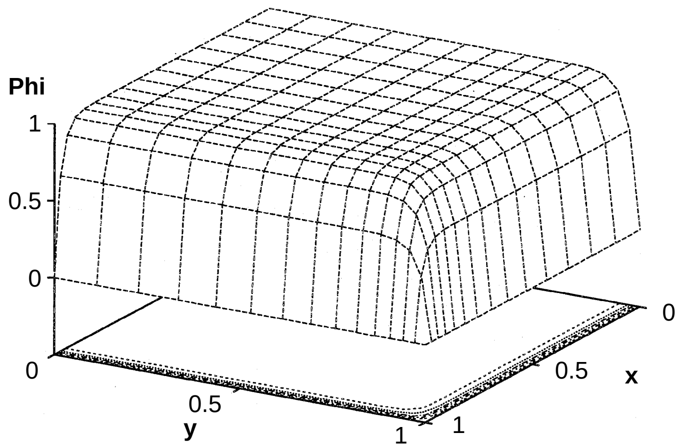

Figure 6.
Surface and contour plot of the HOC solution to 2D test problem on a nonuniform grid

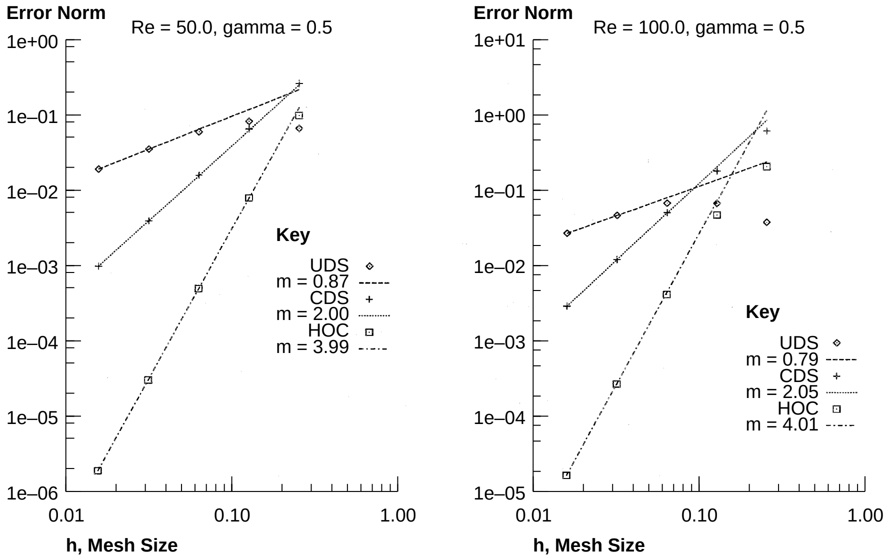

Figure 7. Convergence results for 2D convection diffusion on a nonuniform grid with exact metrics, *Re* = 50 and 100

6. Concluding remarks

We have extended the special class of HOC schemes considered here to include nonuniform grids. When the grid metrics are known analytically, the HOC scheme provides a significant increase in the accuracy of the approximation to the convection diffusion problem solved on a nonuniform grid. For the more common case where the metrics are not known analytically, and the metrics are approximated with central differences, the HOC scheme is degraded to the same convergence rate as the CDS. However, even for this case, the HOC method is more accurate especially when convection is increased. Furthermore, the HOC method with differenced metrics in 1D was seen to suppress oscillations, an important property for a convective transport model.

To maintain $O(h^4)$ accuracy in the HOC scheme, the grid metrics must be approximated to at least $O(h^4)$. This can be done in a manner analogous to the development of the HOC formulation of the governing transport equation, if an auxiliary relation exists which describes the grid mapping. This is often the case when a PDE grid generator has been employed. In lieu of such a relation, we may resort to non-compact difference stencils or other strategies for the metrics to achieve the desired order of accuracy.

In 2D, the general transformation to the computational domain results in the addition of a cross-derivative term and all of the second-order derivatives in the transformed equation have different (and variable) coefficients. Hence the HOC approach becomes much more complicated. However, we have demonstrated that the strategy is viable and tested the approach for graded tensor-product grids in 2D. The further extension to more general irregular structured grids remains an open issue. The methodology presented here applied to a nonorthogonal grid would result in an $O(h^2)$ approximation. However, 1D experiments indicate that such a formulation would suppress artificial oscillations and yield more accurate solutions than more standard $O(h^2)$ schemes, even though the convergence rates are the same.

The accuracy achieved with our HOC scheme is comparable to other high-order finite difference schemes that must use extended stencils or to high-degree (p-type) finite elements. Note that both of these latter schemes involve much larger model stencils. That is, there are more non-zeros per row and the matrix is less tightly banded. For example, bi-cubic elements will generate an $O(h^4)$ scheme but there are now 49 non-zeros per row compared with only nine in our HOC scheme. On the other hand, the p-type schemes are more broadly applicable. One of the major detractions of the higher-order compact schemes is the algebraic difficulty in constructing them for PDEs with variable coefficients in higher dimensions. Symbolic manipulators may eventually alleviate or remove this difficulty. Our recent experience suggests that they are not yet able to do so.

References

Abarbanel, S. and Kumar, A. (1988), "Compact higher-order schemes for the Euler equations", *Journal of Scientific Computing*, Vol. 3, pp. 275-88.

Anderson, D.A., Tannehill, J.C. and Pletcher, R.H. (1984), *Computational Fluid Mechanics and Heat Transfer*, Hemisphere Publishing Corporation, New York, NY.

Boisvert, R.F. (1981), "Families of high order accurate discretizations of some elliptic problems", *SIAM Journal on Scientific and Statistical Computing*, Vol. 2 No. 3, pp. 268-84.

Brandt, A. (1982), "Guide to multigrid development", in Hackbush, W. and Trottenberg, V. (Eds), *Multigrid Methods: Proceedings, Koln-Porz, 1981*, Springer-Verlag, New York, NY, pp. 220-312.

Dennis, S.C.R. and Hudson, J.D. (1989), "Compact h^4 finite difference approximations to operators of Navier-Stokes type", *Journal of Computational Physics*, Vol. 85, pp. 390-416.

Dukowicz, J.K. and Ramshaw, J.D. (1979), "Tensor viscosity method for convection in numerical fluid dynamics", *Journal of Computational Physics*, Vol. 32, pp. 71-9.

Gupta, M.M. *et al.* (1982), "Single-cell high order difference method for steady state advection-diffusion equation", *Proceedings of the Symposium – International Association for Hydraulic Research*, pp. 101-08.

Gupta, M.M., Manohar, R.P. and Stephenson, J.W. (1984), "A single cell high order scheme for the convection-diffusion equation with variable coefficients", *International Journal for Numerical Methods in Fluids*, Vol. 4, pp. 641-51.

Hemker, P.W. (1982), "Mixed defect correction iteration for the accurate solution of the convection diffusion equation", in Hackbush, W. and Trottenberg, U. (Eds), *Multigrid Methods: Proceedings, Koln-Porz, 1981*, Lecture Notes in Mathematics, Springer-Verlag, New York, NY, pp. 485-501.

Johnson, R.W. and MacKinnon, R.J. (1992), "An auxiliary equation method obtaining superconvergent finite element approximations", *Communications in Applied Numerical Methods*, Vol. 8, pp. 99-107.

Leonard, B.P. (1979), "A stable and accurate convective modeling procedure based on quadratic upstream interpolation", *Computer Methods in Applied Mechanics and Engineering*, Vol. 19, pp. 59-98.

Leonard, B.P. and Mokhtari, S. (1990), "Beyond first-order upwinding: the ultra-sharp alternative for non-oscillatory steady-state simulation of convection", *International Journal for Numerical Methods in Engineering,* Vol. 30, pp. 729-66.

Lynch, R.E. and Rice, J.R. (1978), "High accuracy finite difference approximation to solutions of elliptic partial differential equations", *Proceedings of the National Academy of Sciences, USA*, Vol. 75 No. 6, pp. 2541-4.

MacKinnon, R.J. and Carey, G.F. (1989), "Superconvergent derivatives: a Taylor series analysis", *International Journal for Numerical Methods in Engineering*, Vol. 28, pp. 489-509.

MacKinnon, R.J. and Carey, G.F. (1990), "Nodal superconvergence and solution enhancement for a class of finite element and finite difference methods", *SIAM Journal on Scientific and Statistical Computing*, Vol. 11 No. 2, pp. 343-53.

MacKinnon, R.J. and Johnson, R.W. (1991), "Differential equation based representation of truncation errors for accurate numerical simulation", *International Journal for Numerical Methods in Fluids*, Vol. 13, pp. 739-57.

Noye, B.J. (1990), "New third-order finite-difference method for transient one-dimensional advection-diffusion", *Communications in Applied Numerical Methods*, Vol. 6 No. 4, pp. 279-88.

Noye, B.J. and Tan, H.H. (1988), "A third-order semi-implicit finite difference method for solving the one-dimensional convection-diffusion equation", *International Journal for Numerical Methods in Engineering*, Vol. 26 No. 7, pp. 1615-29.

Noye, B.J. and Tan, H.H. (1989), "Finite difference methods for solving the two-dimensional advection-diffusion equation", *International Journal for Numerical Methods in Fluids*, Vol. 9 No. 1, pp. 75-98.

Ribbens, C.J. (1989), "A fast adaptive grid scheme for elliptic partial differential equations", *ACM Transaction on Mathematical Software*, Vol. 15 No. 3, pp. 179-97.

Spotz, W.F. (1991), "Superconvergent finite difference methods with applications to viscous flow", Master's thesis, University of Texas at Austin, TX.

Spotz, W.F. and Carey, G.F. (1995), "High-order compact scheme for the stream-function vorticity equations", *International Journal for Numerical Methods in Engineering*, Vol. 38 No. 20, pp. 3497-512.

Spotz, W.F. and Carey, G.F. (1996), "A high-order compact formulation for the 3D Poisson equation", *Numerical Methods for Partial Differential Equations,* Vol. 12, pp. 235-43.

White, A. (1989), Personal communication, Los Alamos.