

Order of accuracy of QUICK and related convection-diffusion schemes

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This paper explains significant differences in truncation error between finite-difference and finite-volume convection-diffusion schemes. Specifically, the order of accuracy of the QUICK scheme for steady-state convection and diffusion is discussed in detail. Other related convection-diffusion schemes are also considered. The original one-dimensional QUICK scheme written in terms of nodal-point values of the convected variable (with a 1/8-factor multiplying the "curvature" term) is indeed a third-order representation of the finite-volume formulation of the convection operator average across the control volume, written naturally in flux-difference form. An alternative single-point upwind difference scheme (SPUDS) using node values (with a 1/6-factor) is a third-order representation of the finite-difference single-point formulation; this can be written in a pseudo-flux-difference form. These are both third-order convection schemes; however, the QUICK finite-volume convection operator is 33% more accurate than the single-point implementation of SPUDS. Another finite-volume scheme, writing convective fluxes in terms of cell-average values, requires a 1/6-factor for third-order accuracy. For completeness, one can also write a single-point formulation of the convective derivative in terms of cell averages and then express this in pseudo-flux-difference form; for third-order accuracy, this requires a curvature factor of 5/24. Diffusion operators are also considered in both finite-difference and finite-volume formulations. Finite-volume formulations are found to be significantly more accurate. For example, classical second-order central differencing for the second derivative is exactly twice as accurate in a finite-volume formulation as it is in a finite-difference formulation.

Keywords: truncation error, finite-difference, finite-volume, convection, diffusion, QUICK

1. Introduction

The QUICK scheme¹ was introduced in 1979. From time to time since then there appears to have been some controversy regarding the formal order of accuracy of the convection terms. There have been attempts to clarify the situation,^{2,3} but a recent journal article⁴ indicates that the distinction between finite-difference and finite-volume formulations is still not widely understood in the computational-fluid-dynamics (CFD) literature. This paper is a further attempt to correct some of the misunderstandings that have arisen.

First, for definiteness, consider a one-dimensional model problem on a uniform grid of mesh-size h , numerically simulating a (nondimensional) convection-diffusion equation with constant coefficients

$$\frac{\partial \phi}{\partial x} = \frac{1}{Pé} \frac{\partial^2 \phi}{\partial x^2} + S(x) \quad (1)$$

where $Pé$ (= constant > 0) is the macroscopic Péclet number. This simplest model problem has been chosen to highlight the basic differences between finite-difference and finite-volume formulations, without the added complexity of multidimensions, variable coefficients, nonlinearities, and nonuniform grids. The same principles outlined here are also applicable in more general cases, although of course details will be more complicated.

With appropriate boundary conditions, equation (1) represents steady-state one-dimensional convection and diffusion of a scalar with a known source term. A finite-difference numerical approximation of this problem simulates the derivatives involved in equation (1), directly,

$$\left(\frac{\partial \phi}{\partial x} \right)_i = \frac{1}{Pé} \left(\frac{\partial^2 \phi}{\partial x^2} \right)_i + S_i \quad (2)$$

at each nodal grid-point, i . This will be called the single-point (SP) formulation. By contrast, a finite-volume formulation is obtained by integrating equation (1) across a control-volume cell and dividing by h . This gives, for control-volume i ,

$$\left(\frac{\phi_r - \phi_l}{h} \right) = \frac{1}{Pé} \left(\frac{\phi'_r - \phi'_l}{h} \right) + \bar{S}_i \quad (3)$$

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where left and right face-values of the variable and its gradient are indicated, and \bar{S}_i is the control-volume average of the source term at control-volume cell i . This is the operator-average (OA) formulation. Conservation of convective-plus-diffusive flux is guaranteed if the modelled face values and gradients satisfy the uniqueness conditions

$$\phi_l(i) = \phi_r(i - 1) \tag{4}$$

and

$$\phi'_l(i) = \phi'_r(i - 1) \tag{5}$$

Note that equation (3) is an exact equation and not an approximation of equation (2). They are related by (the one-dimensional form of) Gauss' divergence theorem. Similar (but obviously more complicated) exact finite-volume forms are obtained in three dimensions by integrating over the control volume and converting volume integrals into surface integrals using the divergence theorem. This holds similarly in two dimensions.

In order to create numerical algorithms for (approximately) solving equations (2) or (3), one needs to estimate either the derivatives in equation (2) or, alternatively, the face values and gradients appearing in equation (3). Additionally, in making these estimates, one has the choice of using either node values, ϕ_i , or cell averages, $\bar{\phi}_i$. For the operator-average finite-volume equation, the formulation will automatically be in flux-difference form. Numerical models of single-point formulations of derivatives can usually be written as the difference of terms satisfying conservation, thereby generating a pseudo-flux-difference construction. It is important to stress that such schemes are not finite-volume formulations based on equation (3); they are finite-difference formulations based on equation (2), rewritten in the conservative pseudo-flux-difference form.

The one-dimensional QUICK scheme is based on estimating face values and gradients using quadratic upstream interpolation through node values of ϕ located at the center of control-volume cells. For example, at the right face, a parabola is interpolated through ϕ_{i+1} , ϕ_i , and ϕ_{i-1} (for $Pé > 0$), giving the original "1/8-factor" face value

$$\begin{aligned} (\phi_r)^{QUICK} &= \frac{1}{2}(\phi_{i+1} + \phi_i) \\ &\quad - \frac{1}{8}(\phi_{i+1} - 2\phi_i + \phi_{i-1}) \end{aligned} \tag{6}$$

and, for the gradient,

$$(\phi'_r)^{QUICK} = \frac{(\phi_{i+1} - \phi_i)}{h} \tag{7}$$

with left-face quantities obtained by lowering all indices by 1. Substitution of the QUICK formulas into equation (3) gives, using classical Taylor-series analysis,

$$\begin{aligned} &\left[\frac{\phi_r - \phi_l}{h} + \frac{h^3}{16} \phi_i^{(iv)} + O(h^4) \right] \\ &= \frac{1}{Pé} \left[\frac{\phi'_r - \phi'_l}{h} + \frac{h^2}{24} \phi_i^{(iv)} + O(h^4) \right] + \bar{S}_i \end{aligned} \tag{8}$$

In other words, in this finite-volume formulation, the QUICK convection operator average terms are third-order

accurate, whereas the QUICK diffusion operator average terms are only second-order accurate. Thus, the overall QUICK scheme for the convection-diffusion equation gives $O(h^2)$ convergence as the grid is refined. Controversy in the literature concerning the third-order convection term apparently stems from confusing finite-volume and finite-difference formulations. In particular, equation (3) has sometimes been construed as an approximation of equation (2). It is not. It is a perfectly valid (control-volume) equation in its own right.

1.1 Operator-average or single-point formulations

In order to clarify the distinction between finite-volume (operator average) and finite-difference (single point) formulations, consider the Taylor-series formulas

$$\phi(x) = \phi_i + \phi'_i x + \frac{1}{2} \phi''_i x^2 + \frac{1}{6} \phi'''_i x^3 + \dots \tag{9}$$

$$\phi'(x) = \phi'_i + \phi''_i x + \frac{1}{2} \phi'''_i x^2 + \frac{1}{6} \phi^{(iv)}_i x^3 + \dots \tag{10}$$

$$\begin{aligned} &\vdots \\ \phi^{(n)}(x) &= \phi_i^{(n)} + \phi_i^{(n+1)} x + \frac{1}{2} \phi_i^{(n+2)} x^2 \\ &\quad + \frac{1}{6} \phi_i^{(n+3)} x^3 + \dots \end{aligned} \tag{11}$$

Now compute finite-volume formulas by subtracting the Taylor-expansions written for $x = h/2$ and $x = -h/2$, giving

$$\begin{aligned} \frac{\phi_r^{(n)} - \phi_l^{(n)}}{h} &= \phi_i^{(n+1)} + \frac{h^2}{2^2 3!} \phi_i^{(n+3)} + \frac{h^4}{2^4 5!} \phi_i^{(n+5)} \\ &\quad + \frac{h^6}{2^6 7!} \phi_i^{(n+7)} + \dots \end{aligned} \tag{12}$$

This formula is also valid for negative n (representing integration); in particular, for $n = -1$, the control-volume cell-average of the transported scalar itself is given by

$$\begin{aligned} \bar{\phi}_i &= \frac{1}{h} \int_{-h/2}^{h/2} \phi(x) dx \\ &= \phi_i + \frac{h^2}{24} \phi''_i + \frac{h^4}{1920} \phi_i^{(iv)} + \dots \end{aligned} \tag{13}$$

The expression on the left side of equation (12) represents the control-volume OA of the $(n + 1)$ th derivative, whereas the first term on the right is the SP form. Note that the difference between the two always involves an $O(h^2)$ quantity. This is an important point that is the key to clarifying the confusion that has arisen in the literature. If a finite-volume (OA) discrete operator is viewed as an finite-difference (SP) term, there is an $O(h^2)$ discrepancy between the two. This does not affect the leading truncation error of first-order schemes. Second-order schemes show a change in the numerical value of the h^2 coefficient. But a third (or higher) order OA scheme is only second-order accurate when viewed as an SP scheme, and vice versa. This is apparently why the QUICK scheme has been so controversial.

2. Third-order-accurate steady transport

In a recent paper,⁴ Johnson and MacKinnon attempted to clarify the distinction between finite-difference and finite-volume formulations. Unfortunately, their conclusions are exactly the reverse of the true situation. They claim, in particular, that the QUICK(1/8) scheme is only a second-order accurate finite-volume convection scheme. For example (using here "left-right" rather than "east-west"), Johnson and MacKinnon's equation (4) for the QUICK(1/8) convection scheme is

$$\frac{\phi_r - \phi_l}{h} = \frac{3\phi_{i+1} + 3\phi_i - 7\phi_{i-1} + \phi_{i-2}}{8h} - \frac{h^2}{16} (\phi_r''' - \phi_l''') + \text{HOT} \quad (14)$$

This is correct as written; but Johnson and MacKinnon seem to imply, quoting Bradley et al.,⁵ that this represents an $O(h^2)$ -accurate operator. First of all, from equation (12), with $n = 3$, the leading truncation error is

$$\begin{aligned} \frac{h^2}{16} (\phi_r''' - \phi_l''') &= \frac{h^3}{16} \left(\frac{\phi_r''' - \phi_l'''}{h} \right) \\ &= \frac{h^3}{16} \phi_i^{(iv)} + \frac{h^5}{384} \phi_i^{(vi)} + \dots \end{aligned} \quad (15)$$

Equation (14) is equivalent to the left side of equation (8), showing the QUICK(1/8) convection term indeed to be a third-order accurate finite-volume OA formulation of the term $(\phi_r - \phi_l)/h$. Second, it must be stressed that the discrete operator in equation (14) is not intended to be an SP numerical model of ϕ'_i . If it is considered to be, as in Ref. 4's equation (5), it will appear to be $O(h^2)$ accurate; this is easily seen from equation (12), with $n = 0$.

Johnson and MacKinnon claim to demonstrate the "second"-order accuracy of the QUICK(1/8) convection terms by giving a numerical example of a simple convection-diffusion problem with a known exact solution, using a fourth-order accurate diffusion operator

$$\phi_i'' = \frac{-\phi_{i+2} + 16\phi_{i+1} - 30\phi_i + 16\phi_{i-1} - \phi_{i-2}}{12h^2} + O(h^4) \quad (16)$$

the strategy being that the grid convergence will be dominated by the lower-order convection term. As is well known,⁶ this is indeed a fourth-order finite-difference SP approximation of the second-derivative at point i , consistent with a quartic polynomial interpolated through node points: ϕ_{i-2} , ϕ_{i-1} , ϕ_i , ϕ_{i+1} , and ϕ_{i+2} . However, this is not what is being modelled in a finite-volume formulation. Rather, to be consistent, according to equation (3), one should model the operator average across the control volume. The appropriate fourth-order finite-volume formula is

$$\begin{aligned} \frac{\phi'_r - \phi'_l}{h} &= \frac{-\phi_{i+2} + 28\phi_{i+1} - 52\phi_i + 28\phi_{i-1} - \phi_{i-2}}{24h^2} \\ &+ O(h^4) \end{aligned} \quad (17)$$

More specifically, the fourth-order right-face gradient can be represented by

$$[\phi'_r]_{4th} = \frac{\phi_{i+1} - \phi_i}{h} - \frac{\phi_{i+2} - 3\phi_{i+1} + 3\phi_i - \phi_{i-1}}{24h} \quad (18)$$

obtained by interpolating a cubic polynomial through node points: ϕ_{i-1} , ϕ_i , ϕ_{i+1} , and ϕ_{i+2} .

The $O(h^2)$ convergence reported by Johnson and MacKinnon using QUICK(1/8) for convection and equation (16) for diffusion occurs because their diffusion operator is only $O(h^2)$ accurate in a finite-volume formulation. This can be seen immediately from equation (12), written for $n = 1$:

$$\frac{\phi'_r - \phi'_l}{h} = \phi_i'' + \frac{h^2}{24} \phi_i^{(iv)} + \frac{h^4}{1920} \phi_i^{(vi)} + \dots \quad (19)$$

3. Numerical example

The numerical example used by Johnson and MacKinnon is (with a slight change in notation)

$$\frac{d\phi}{dx} - \frac{1}{\text{Pé}} \frac{d^2\phi}{dx^2} = 0 \quad (20)$$

with boundary conditions on the nodal values

$$\phi(0) = 0 \quad \phi(1) = 1 \quad (21)$$

The exact solution is

$$\phi(x) = \frac{e^{\text{Pé}x} - 1}{e^{\text{Pé}} - 1} \quad (22)$$

Step sizes of 1/4, 1/8, 1/16, 1/32, and 1/64 are used, and $\text{Pé} = 4$. In the current formulation, pseudonode values are required beyond each end of the physical domain. For the purposes of this numerical test, these are taken here to be exact values given by

$$\phi_{-1} = \frac{e^{-4h} - 1}{e^4 - 1} \quad (23)$$

and

$$\phi_{N+1} = \frac{e^{4(1+h)} - 1}{e^4 - 1} \quad (24)$$

3.1 Exact derivatives and fluxes

In order to investigate the effect of individual modelled terms, it is instructive to compute exact derivatives and fluxes from the known analytical solution. For example, errors introduced solely by modelled convection terms can be studied in isolation by using exact diffusion terms and vice versa. From equation (22), the first and second derivatives are

$$\frac{d\phi}{dx} = \frac{\text{Pé} e^{\text{Pé}x}}{e^{\text{Pé}} - 1} \quad (25)$$

and

$$\frac{d^2\phi}{dx^2} = \frac{P\acute{e}^2 e^{P\acute{e}x}}{e^{P\acute{e}} - 1} \quad (26)$$

By integrating equation (20) from $(x - h/2)$ to $(x + h/2)$ and dividing by h , the (exact) control-volume formation is

$$\left(\frac{\phi_r - \phi_l}{h}\right) - \frac{1}{P\acute{e}} \left(\frac{\phi'_r - \phi'_l}{h}\right) = 0 \quad (27)$$

where

$$\phi_l(x) = \phi_r(x - h) \quad (28)$$

and

$$\phi'_l(x) = \phi'_r(x - h) \quad (29)$$

By defining the convective-plus-diffusive flux at any point as

$$F(x) = \frac{\phi(x) - \phi'(x)/P\acute{e}}{h} \quad (30)$$

equation (27) can be written in flux-difference form across any control-volume cell of width h as

$$F_r(x) - F_l(x) = 0 \quad (31)$$

where the exact convective-plus-diffusive fluxes are

$$F_r(x) = \frac{1}{h} \left[\frac{(e^{P\acute{e}x} e^{P\acute{e}h/2} - 1)}{e^{P\acute{e}} - 1} - \frac{e^{P\acute{e}x} e^{P\acute{e}h/2}}{e^{P\acute{e}} - 1} \right] \quad (32)$$

and

$$F_l(x) = \frac{1}{h} \left[\frac{(e^{P\acute{e}x} e^{-P\acute{e}h/2} - 1)}{e^{P\acute{e}} - 1} - \frac{e^{P\acute{e}x} e^{-P\acute{e}h/2}}{e^{P\acute{e}} - 1} \right] \quad (33)$$

introducing the grid Péclet number, $P\acute{e}_\Delta = hP\acute{e}$. Note that conservation is guaranteed, since $F_l(x) = F_r(x - h)$.

3.2 Evaluation of discrete operators

With a uniform grid of step-size h and a control volume centered at x_i , a numerical model of the convective flux can be tested by using a hybrid formulation of equation (30)

$$F_r^{HYB}(x_i) = \frac{1}{h} \left[\phi_r^{model} - \frac{e^{P\acute{e}x_i} e^{P\acute{e}h/2}}{e^{P\acute{e}} - 1} \right] \quad (34)$$

and, assuming the numerical model to be conservative,

$$F_l^{HYB}(x_i) = F_r^{HYB}(x_i - h) \quad (35)$$

If the modelled face values, ϕ_r^{model} and ϕ_l^{model} are written in terms of nodal values of ϕ

$$\phi_i = \phi(x_i) \quad (36)$$

a solution of the flux-difference equation

$$F_r^{HYB}(x_i) - F_l^{HYB}(x_i) = 0 \quad (37)$$

Table 1. Grid-refinement study of the model convection-diffusion equation, using a finite-volume flux-difference OA formulation, with exact diffusive fluxes calculated from the analytical solution. Two convection schemes are compared. Values shown are those of the node-point error at $x = 0.75$.

h^{-1}	QUICK(1/8)	SPUDS(1/6)
4	$-3.93435739 \times 10^{-2}$	$-1.33129698 \times 10^{-2}$
8	$-9.24652759 \times 10^{-4}$	$+3.72661451 \times 10^{-4}$
16	$-2.75420514 \times 10^{-4}$	$+4.77048555 \times 10^{-4}$
32	$-4.12098809 \times 10^{-5}$	$+1.76208352 \times 10^{-4}$
64	$-5.30547084 \times 10^{-6}$	$+5.08534128 \times 10^{-5}$
Rate	$O(h^3)$	$O(h^2)$

then gives the computed ϕ_i values corresponding to the particular convection model, treating the diffusive fluxes exactly. The node-point error is then, using equation (22),

$$NPE_i = \phi_i(\text{computed}) - \frac{e^{P\acute{e}x_i} - 1}{e^{P\acute{e}} - 1} \quad (38)$$

A grid-refinement study (with $h^{-1} = 4, 8, 16, 32,$ and 64) then shows the true convergence rate of the convective model in isolation. The rate, R , can be obtained from

$$\frac{|NPE_i(h)|}{|NPE_{2i}(h/2)|} = 2^R \quad (39)$$

and should approach an asymptotic value as h becomes smaller and smaller.

Standard QUICK scheme. —Equation (6) for the right face value is rewritten here for convenience

$$\begin{aligned} (\phi_r)^{QUICK} &= \frac{1}{2}(\phi_{i+1} + \phi_i) \\ &\quad - \frac{1}{8}(\phi_{i+1} - 2\phi_i + \phi_{i-1}) \end{aligned} \quad (40)$$

with the left face value given by

$$\begin{aligned} (\phi_l)^{QUICK} &= \frac{1}{2}(\phi_i + \phi_{i-1}) \\ &\quad - \frac{1}{8}(\phi_i - 2\phi_{i-1} + \phi_{i-2}) \end{aligned} \quad (41)$$

Using exact diffusive fluxes as described above, the results in the QUICK(1/8) column of *Table 1* show that the node-point error at $x = 0.75$ converges at a rate of $O(h^3)$.

The SPUDS formulation. —An alternate formulation, recommended by a number of researchers,⁴ is based on a single-point upwind difference scheme modelling the derivative, i.e.,

$$\left(\frac{d\phi}{dx}\right)_i^{SPUDS} = \frac{2\phi_{i+1} + 3\phi_i - 6\phi_{i-1} + \phi_{i-2}}{6h} \quad (42)$$

This is then written in pseudo-flux-difference form

$$\left(\frac{d\phi}{dx}\right)_i^{SPUDS} = \frac{(\phi_r^*)^{SPUDS} - (\phi_l^*)^{SPUDS}}{h} \quad (43)$$

where

$$\begin{aligned} (\phi_r^*)^{SPUDS} &= \frac{1}{2}(\phi_{i+1} + \phi_i) \\ &\quad - \frac{1}{6}(\phi_{i+1} - 2\phi_i + \phi_{i-1}) \end{aligned} \quad (44)$$

and

$$(\phi'_i)^{SPUDS} = \frac{1}{2}(\phi_i + \phi_{i-1}) - \frac{1}{6}(\phi_i - 2\phi_{i-1} + \phi_{i-2}) \quad (45)$$

Johnson and MacKinnon call this a "finite-volume" formulation.⁴ When this convection model is used in equation (37), using the exact diffusive flux of equation (34), the node-point error asymptotes to a second-order trend, as seen in the SPUDS(1/6) column of Table 1. Clearly, SPUDS represents a second-order finite-volume formulation of the convective term.

However, SPUDS was not really designed to simulate $(\phi_r - \phi_l)/h$. Instead, it is a model of the single-point differential formulation given by equation (20), which is then written in pseudo-flux-difference form. Testing the scheme with the exact finite-volume form of the diffusive fluxes is, therefore, inappropriate. A proper test would use the exact second derivative of equation (26) in pseudo-flux-difference form. This can be achieved by writing

$$\left(\frac{d^2\phi}{dx^2}\right)_i = \frac{(\phi'_r)^* - (\phi'_l)^*}{h} \quad (46)$$

where (for the particular model problem under consideration) the exact right pseudo-gradient is

$$(\phi'_r)^* = \left(\frac{P\epsilon e^{P\epsilon x_i} e^{P\Delta/2}}{e^{P\epsilon} - 1}\right) \left(\frac{P\Delta/2}{\sinh P\Delta/2}\right) \quad (47)$$

and the exact left pseudo-gradient is obtained by replacing x_i by $(x_i - h)$. When these formulas are used in the hybrid flux formulation, the node-point error shows a third-order trend, as seen in the SPUDS(1/6) column of Table 2.

As a matter of interest, using the QUICK(1/8) convection scheme in combination with the single-point exact diffusion operator gives an $O(h^2)$ trend. This is shown in the QUICK(1/8) column of Table 2. This is to be expected from equation (12), since the finite-volume QUICK(1/8) scheme is now being used out of context in a single-point formulation, just as the SPUDS(1/6) scheme is $O(h^2)$ when used in a finite-volume formulation.

Of the two third-order convection schemes considered—the QUICK(1/8) finite-volume formulation in Table 1 and the SPUDS(1/6) formulation in Table 2—note that

Table 2. Grid-refinement study of the convection-diffusion equation, using the SP differential equation expressed in pseudo-flux-difference form, with exact diffusion terms calculated from the analytical solution. Two convection schemes are compared. Values shown are those of the node-point error at $x = 0.75$.

h^{-1}	SPUDS(1/6)	QUICK(1/8)
4	$-4.35438228 \times 10^{-2}$	$-7.45209055 \times 10^{-2}$
8	$-1.86968335 \times 10^{-3}$	$-2.38132421 \times 10^{-3}$
16	$-3.97474350 \times 10^{-4}$	$-1.07787069 \times 10^{-3}$
32	$-5.50611000 \times 10^{-5}$	$-2.71242977 \times 10^{-4}$
64	$-7.06282736 \times 10^{-6}$	$-6.32202472 \times 10^{-5}$
Rate	$O(h^3)$	$O(h^2)$

Table 3. Grid-refinement study of diffusion schemes using exact convection terms. Node-point errors are shown at $x = 0.75$. In column 1, the QUICK finite-volume OA scheme is used. Column 2 gives results for classical central differencing using an SP formulation.

h^{-1}	QUICK	CDS
4	$+1.59466830 \times 10^{-2}$	$+3.12478024 \times 10^{-2}$
8	$+4.07354976 \times 10^{-3}$	$+8.10497409 \times 10^{-3}$
16	$+1.02395148 \times 10^{-3}$	$+2.04524126 \times 10^{-3}$
32	$+2.56328047 \times 10^{-4}$	$+5.12489289 \times 10^{-4}$
64	$+6.38006991 \times 10^{-5}$	$+1.27591015 \times 10^{-4}$
Rate	$O(h^2)$	$O(h^2)$

the finite-volume formulation is asymptotically 33% more accurate. The reason for this is explained by a formal discretization error analysis in the Appendix.

3.3 Diffusion models

For evaluating numerical models of diffusion terms, the hybrid finite-volume flux is written

$$F_r^{HYB}(x_i) = \frac{1}{h} \left[\frac{(e^{P\epsilon x_i} e^{P\Delta/2} - 1)}{(e^{P\epsilon} - 1)} - \frac{(\phi'_r)_{\text{model}}}{P\epsilon} \right] \quad (48)$$

with a corresponding formula, $F_l^{HYB}(x_i) = F_r^{HYB}(x_i - h)$ for the left face. If a single-point formulation is used, written in pseudo-flux-difference form, then the appropriate formula (for the current exponential solution) is

$$F_r^*(x_i) = \frac{1}{h} \left[\frac{P\Delta(e^{P\epsilon x_i} e^{P\Delta/2} - 1)}{(e^{P\epsilon} - 1)2 \sinh P\Delta/2} - \frac{(\phi'_r)_{\text{model}}^*}{P\epsilon} \right] \quad (49)$$

3.4 QUICK diffusion flux

Interpolating a parabola through node values ϕ_{i-1} , ϕ_i , and ϕ_{i+1} , on a uniform grid, leads to

$$(\phi'_r)^{QUICK} = \frac{\phi_{i+1} - \phi_i}{h} \quad (50)$$

Because of a geometric property of the parabola, this is indistinguishable from linear interpolation between node values ϕ_i and ϕ_{i+1} . When used with a finite-volume formulation of the exact convection terms, equation (48), this leads to the $O(h^2)$ convergence shown in the QUICK column of Table 3.

3.5 Classical central differencing

If the second derivative at point i is approximated by the second central difference

$$\left(\frac{d^2\phi}{dx^2}\right)_i^{\text{model}} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{h^2} \quad (51)$$

Table 4. Grid-refinement study of diffusion schemes, using a finite-volume flux-difference OA formulation, with exact convective fluxes calculated from the analytical solution. Two diffusion schemes are compared. Values shown are those of the node-point error at $x = 0.75$.

h^{-1}	Equation (17)	Equation (16)
4	$-1.74276854 \times 10^{-3}$	$-1.70401744 \times 10^{-2}$
8	$-1.12027932 \times 10^{-4}$	$-4.02705160 \times 10^{-3}$
16	$-7.10364599 \times 10^{-6}$	$-1.00591394 \times 10^{-3}$
32	$-4.47274921 \times 10^{-7}$	$-2.53235117 \times 10^{-4}$
64	$-2.79314528 \times 10^{-8}$	$-6.33685964 \times 10^{-5}$
Rate	$O(h^4)$	$O(h^2)$

the corresponding pseudo-flux-difference formulation involves the pseudo-gradient

$$(\phi'_r)^* = \frac{\phi_{i+1} - \phi_i}{h} \quad (52)$$

which, of course, is superficially identical to the QUICK formulation of equation (50). But, in this case, the appropriate (pseudo-) convective flux is given by equation (49). The grid convergence behavior is, therefore, not identical to that of the QUICK diffusive formulation. As seen in the CDS column of Table 3, single-point classical second-order central differencing for diffusion asymptotically generates errors exactly twice as large as the identical operator used in a finite-volume formulation, using exact convective terms in each case. The reason for this is seen in the Appendix.

3.6 Fourth-order diffusion terms

Consider the diffusion operators given by equations (16) and (17). Table 4 shows the finite-volume formulation using exact convective fluxes from equation (48). As expected, equation (17) shows an $O(h^4)$ trend, whereas equation (16)—being used out of context—is only $O(h^2)$, according to equation (12).

Alternatively, Table 5 shows the single-point formulation using the same diffusion operators together with equation (49) for convection. In this case, the convergence is reversed, as expected, since now equation (17) is being used out of context.

Table 5. Grid-refinement study of diffusion schemes, using the SP differential equation expressed in pseudo-flux-difference form, with exact convection terms calculated from the analytical solution. Two diffusion schemes are compared. Values shown are those of the node-point error at $x = 0.75$.

h^{-1}	Equation (16)	Equation (17)
4	$-3.81023176 \times 10^{-3}$	$+1.24370324 \times 10^{-2}$
8	$-2.56261277 \times 10^{-4}$	$+3.78389793 \times 10^{-3}$
16	$-1.65684268 \times 10^{-5}$	$+9.97608855 \times 10^{-4}$
32	$-1.05202438 \times 10^{-6}$	$+2.53650099 \times 10^{-4}$
64	$-6.59600528 \times 10^{-8}$	$+6.35095680 \times 10^{-5}$
Rate	$O(h^4)$	$O(h^2)$

Table 6. Grid-refinement study of the convection-diffusion equation, using a finite-volume flux-difference (or pseudo-flux-difference) formulation of two schemes: (i) the standard QUICK convection-diffusion scheme; and (ii) the SPUDS convection operator together with CDS for diffusion. Values shown are those of the node-point error at $x = 0.75$.

h^{-1}	Standard QUICK	SPUDS + CDS
4	$+9.96622011 \times 10^{-4}$	$+7.58488389 \times 10^{-3}$
8	$+1.25198293 \times 10^{-3}$	$+3.87320949 \times 10^{-3}$
16	$+5.56979450 \times 10^{-4}$	$+1.30280308 \times 10^{-3}$
32	$+1.74361676 \times 10^{-4}$	$+3.73713298 \times 10^{-4}$
64	$+4.82503616 \times 10^{-5}$	$+9.97187451 \times 10^{-5}$
Rate	$O(h^2)$	$O(h^2)$

Note that the fourth-order single-point diffusion operator in Table 5 generates errors more than twice as large as those of the fourth-order finite-volume operator in Table 4. This, again, appears to suggest that a true finite-volume formulation is likely to be more accurate than the corresponding single-point scheme of the same formal order of accuracy.

3.7 Convection-diffusion schemes

For reference, Table 6 shows a grid-refinement study of two convection-diffusion schemes: (i) the standard finite-volume QUICK scheme, using equation (6) for convection and equation (50) for diffusion; and (ii) the SPUDS scheme, equation (44), for convection, together with classical second-order central-differencing, equation (52), for diffusion. Both schemes are $O(h^2)$ because of the dominance of the diffusion terms at the fine-grid end of the spectrum. Note, however, that the SPUDS + CDS scheme asymptotically generates errors twice as large as those of the standard finite-volume QUICK formulation. This is clarified in the Appendix.

4. Cell averages as dependent variables

Up until this point in the discussion, modelled derivatives and fluxes have been written in terms of nodal point values of the dependent variable. But many CFD schemes—especially finite-volume formulations—treat the cell averages as the dependent variables, writing the convective and diffusive fluxes directly in terms of the ϕ 's. (It is also theoretically possible to write single-point formulations in terms of cell averages, although this does not appear to have ever been proposed in the CFD literature.) Note that the distinction only occurs at third order and above; for first- and second-order schemes, $\bar{\phi}_i \equiv \phi_i$.

From the analytical solution to the model problem being studied, the exact formula for the cell average, defined in equation (13), can be found as

$$\bar{\phi}_i = \frac{e^{Pe x_i} [(\sinh P_\Delta/2)/(P_\Delta/2)] - 1}{e^{Pe} - 1} \quad (53)$$

The only difference between this and the exact nodal point solution for ϕ_i , equation (22), is the appearance of the

Table 7. Comparison of exact node-point values, ϕ_i , with exact cell-average values, $\bar{\phi}_i$, for the model convection-diffusion problem with $h = 1/8$.

x_i	ϕ_i	$\bar{\phi}_i$
0	0.0	0.000194956
0.125	0.012103427	0.012424854
0.25	0.032058603	0.032588548
0.375	0.064959128	0.065832859
0.5	0.119202922	0.120643461
0.625	0.208635820	0.211010867
0.75	0.356085740	0.360001531
0.875	0.599189560	0.605645608
1	1.0	1.010644223

hyperbolic-sine factor (in square brackets). For a given Pé, this factor depends on the grid size; Table 7 shows ϕ_i and $\bar{\phi}_i$ values for $h = 1/8$. Note that the sinh factor has a Taylor expansion given by

$$\frac{\sinh P_\Delta/2}{P_\Delta/2} = 1 + \frac{P_\Delta^2}{24} + \frac{P_\Delta^4}{1920} + \dots \quad (54)$$

which should be compared with equation (13), for example.

4.1 Subcell interpolation

Given a set of $\bar{\phi}$ (cell-average) values, one would like to interpolate a subcell $\phi(x)$ satisfying equation (13). This can be done quite easily by introducing a discrete integral variable, ψ_i , defined by

$$\psi_i = \psi_{i-1} + h\bar{\phi}_i \quad (55)$$

where it is understood that ψ_i values occur at the right face of the corresponding cell i . An interpolation, $\psi(x)$, collocated at ψ_i values can then be differentiated to give $\phi(x)$:

$$\phi(x) = \frac{d\psi(x)}{dx} \quad (56)$$

automatically satisfying equation (13), no matter what type of interpolation is used for $\psi(x)$, provided the collocation conditions

$$\psi(x_i + h/2) = \psi_i \quad \text{for all } i \quad (57)$$

are satisfied, where x_i is located at the center of cell i .

For example, piece-wise polynomial interpolation can be used for interpolating $\psi(x)$ over each cell i . In this case, discontinuities in slope occur in $\psi(x)$ at cell faces; these correspond to discontinuities in value in $\phi(x)$ across cell faces.

4.2 Third-order finite-volume convection terms

Just as with the QUICK(1/8) finite-volume convection scheme using nodal point values, the corresponding third-order cell-average formula is based on local (piece-wise)

quadratic interpolation of $\phi(x)$. This requires piece-wise cubic interpolation of $\psi(x)$. For cell i , a symmetrically located cubic is interpolated by collocation through ψ_{i-2} , ψ_{i-1} , ψ_i , and ψ_{i+1} , giving

$$\begin{aligned} \psi(\xi) = & \psi_i + \left(\frac{\psi_{i+1} - \psi_{i-1}}{2} \right. \\ & \left. - \frac{\psi_{i+1} - 3\psi_i + 3\psi_{i-1} - \psi_{i-2}}{6} \right) \left(\frac{\xi}{h} \right) \\ & + \left(\frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{2} \right) \left(\frac{\xi}{h} \right)^2 \\ & + \left(\frac{\psi_{i+1} - 3\psi_i + 3\psi_{i-1} - \psi_{i-2}}{6} \right) \left(\frac{\xi}{h} \right)^3 \end{aligned} \quad (58)$$

over the range: $-h \leq \xi \leq 0$, where $\xi = x - (x_i + h/2)$. From its definition, equation (56), the subcell interpolation across cell i is then given by the quadratic

$$\begin{aligned} \phi(\xi) = & \frac{1}{2}(\bar{\phi}_{i+1} + \bar{\phi}_i) - \frac{1}{6}(\bar{\phi}_{i+1} - 2\bar{\phi}_i + \bar{\phi}_{i-1}) \\ & + (\bar{\phi}_{i-1} - \bar{\phi}_i) \left(\frac{\xi}{h} \right) \\ & + \frac{1}{2}(\bar{\phi}_{i+1} - 2\bar{\phi}_i + \bar{\phi}_{i-1}) \left(\frac{\xi}{h} \right)^2 \end{aligned} \quad (59)$$

For steady flow (with $\text{Pé} > 0$), the right face value of cell i is given by

$$\begin{aligned} \phi_r(i) = \phi(\xi = 0) = & \frac{1}{2}(\bar{\phi}_{i+1} + \bar{\phi}_i) \\ & - \frac{1}{6}(\bar{\phi}_{i+1} - 2\bar{\phi}_i + \bar{\phi}_{i-1}) \end{aligned} \quad (60)$$

This "1/6" formula in terms of cell averages is consistent with the "1/8" formula using nodal point values. This can be seen by using equation (59) to evaluate ϕ_i in terms of the $\bar{\phi}$'s:

$$\phi_i = \phi(\xi = -h/2) = \bar{\phi}_i - \frac{1}{24}(\bar{\phi}_{i+1} - 2\bar{\phi}_i + \bar{\phi}_{i-1}) \quad (61)$$

and noting that $1/6 = 1/8 + 1/24$.

Table 8. Grid refinement study of the finite-volume convection scheme corresponding to equation (60), based on cell-average values and using exact diffusive fluxes. The cell-average error is shown together with the corresponding node-point error using equation (61).

h^{-1}	CAE (@ $x = 0.75$)	NPE (@ $x = 0.75$)
4	$-4.53809633 \times 10^{-2}$	$-5.18134013 \times 10^{-2}$
8	$-1.88922017 \times 10^{-3}$	$-1.90618632 \times 10^{-2}$
16	$-3.98510249 \times 10^{-4}$	$-4.48060981 \times 10^{-4}$
32	$-5.50969540 \times 10^{-5}$	$-6.76253568 \times 10^{-5}$
64	$-7.06397697 \times 10^{-6}$	$-1.01264031 \times 10^{-5}$
Rate	$O(h^3)$	$O(h^3)$

Table 9. Grid refinement study of the SP convection scheme corresponding to equation (64), based on cell average values and using exact diffusion terms. The cell-average error is shown together with the corresponding node-point error using equation (61).

h^{-1}	CAE (@ $x = 0.75$)	NPE (@ $x = 0.75$)
4	$-4.86965236 \times 10^{-2}$	$-5.52922960 \times 10^{-2}$
8	$-2.86590535 \times 10^{-3}$	$-2.90394004 \times 10^{-3}$
16	$-5.11359278 \times 10^{-4}$	$-5.62692325 \times 10^{-4}$
32	$-6.86685845 \times 10^{-5}$	$-8.11969093 \times 10^{-5}$
64	$-8.81228514 \times 10^{-6}$	$-1.18744119 \times 10^{-5}$
Rate	$O(h^3)$	$O(h^3)$

4.3 Grid-refinement using cell averages

If equation (60) for $\phi_r(i)$ and the corresponding formula for ϕ_l given by conservation, $\phi_l(i) = \phi_r(i - 1)$, are used together with exact diffusive fluxes, using equations (34) and (35), solution of the resulting difference equation will, of course, generate approximate ϕ_i values (as opposed to $\bar{\phi}_i$ values). These should be compared with the corresponding exact $\bar{\phi}_i$ values by introducing the cell-average error

$$CAE_i = \bar{\phi}_i(\text{computed}) - \bar{\phi}_i(\text{exact}) \tag{62}$$

using equation (53) for $\bar{\phi}_i(\text{exact})$. Table 8 shows CAE values at $x = 0.75$ for convective modelling errors using equation (60) together with exact diffusive fluxes. As expected from the quadratic construction of face values, this is a third-order accurate scheme. One can, of course, retrieve node values by using equation (61). The corresponding NPE at $x = 0.75$ is also shown in the table.

4.4 Single-point formulation using cell averages

For completeness, the single-point formulation using cell averages should be considered. To achieve third-order accuracy, this requires an upwind-weighted cubic subcell reconstruction of $\phi(x)$ corresponding to a quartic piecewise polynomial interpolation of $\psi(x)$, collocated at ψ_{i-3} , ψ_{i-2} , ψ_{i-1} , ψ_i , and ψ_{i+1} (for $Pé > 0$). This gives

$$\left(\frac{d\phi}{dX}\right)_i^{\text{model}} = \frac{7\bar{\phi}_{i+1} + 15\bar{\phi}_i - 27\bar{\phi}_{i-1} + 5\bar{\phi}_{i-2}}{24h} \tag{63}$$

This can be expressed in pseudo-flux-difference form by identifying

$$\phi_r^*(i) = \frac{1}{2}(\bar{\phi}_{i+1} + \bar{\phi}_i) - \frac{5}{24}(\bar{\phi}_{i+1} - 2\bar{\phi}_i + \bar{\phi}_{i-1}) \tag{64}$$

with $\phi_l^*(i) = \phi_r^*(i - 1)$, as usual. Table 9 shows the corresponding grid convergence of CAE and NPE at $x = 0.75$.

5. Conclusion

In constructing convection-diffusion schemes, there are four general categories. First, one can choose to model

first and second derivatives at a single point; this is the SP formulation. Alternatively, one can choose to model the face values and gradients in a finite-volume formulation; this is the operator-average, or OA, formulation. Each of these formulations can use either nodal point values or cell-average values of the dependent variable. Control-volume formulations are automatically in conservative flux-difference form. The two SP formulations can also usually be written in a pseudo-flux-difference form; in this case, conservation is satisfied even though the modelled "fluxes" do not represent the true physical fluxes. When working with third (or higher)-order convection methods, it is important to model all terms in the equation in the same manner (i.e., either all SP or all OA); a mixed formulation is condemned to (at best) second-order accuracy, no matter how accurate the individual terms.

For a model problem with a known analytical solution, the order of accuracy of the convection terms in isolation can be studied in a grid refinement test, using exact diffusion terms (and vice versa). Tests of this type showed that, for methods using nodal point values:

- QUICK(1/8) is $O(h^3)$ accurate in an OA formulation but only $O(h^2)$ accurate in an SP formulation.
- SPUDS(1/6) is $O(h^3)$ accurate in an SP formulation but only $O(h^2)$ accurate in an OA formulation.

For methods using cell-average values as dependent variables:

- The "1/6" formula gives $O(h^3)$ convergence in an OA formulation.
- An SP formulation requires a "5/24" factor for $O(h^3)$ accuracy.

In general, finite-volume formulations are considerably more accurate than the corresponding finite-difference formulation of the same formal order. For example, the QUICK(1/8) third-order finite-volume convection scheme is 33% more accurate than the SPUDS(1/6) third-order finite-difference scheme. Similarly, the QUICK(1/8) convection-diffusion scheme in a finite-volume formulation is asymptotically twice as accurate as using SPUDS(1/6) for convection with CDS for diffusion in a single-point formulation, although both schemes are formally only second-order accurate because of the dominance of the diffusion terms in the fine-grid limit.

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Appendix A: Relationship between truncation error and discretization error

In the following analysis, it is assumed that the problem is linear, steady, and one-dimensional involving a uniform spatial grid of mesh-size h . Generalization of these conditions are relatively straightforward. The analysis establishes the (often taken for granted) fact that discretization

error in the solution is of the same order of accuracy as truncation error in the operator in a single-point formulation. The same is true of finite-volume formulations.

Single-point formulation

Consider a linear operator involving derivatives of various orders at a single point. This (exact) differential operator is represented by L . Assume that $U(x)$ is the exact, $O(1)$, solution of the exact differential equation

$$L(U) = S(x) \tag{A1}$$

where $S(x)$ is a known source term. Now consider a discrete operator representing a numerical approximation to the single-point differential operator; this is represented by D . Assume that u_i is the exact nodal-point solution of the approximate numerical difference equation, defined at nodal points i , i.e.,

$$D(u_i) = S_i \tag{A2}$$

where $S_i = S(x_i)$ is known exactly (an approximate S_i will, of course, introduce source-term errors).

To define the truncation error of the numerical operator, assume that $v(x)$ is a test function possessing all derivatives. Then the truncation error can be defined as the difference between the approximate and exact operators, operating on v at the nodal point i :

$$TE_{SP}(v)|_i = D(v)|_i - L(v)|_i \tag{A3}$$

By making Taylor series expansions of the terms in $D(v)|_i$, the truncation error will be found to depend on h , as follows

$$TE_{SP}(v)|_i = P(v)|_i h^p + HOT = O(h^p) \tag{A4}$$

where $P(v)$ involves derivatives of v , and p is an integer. Note that using U as the test function in equation (A3) gives

$$D(U)|_i = L(U)|_i + TE_{SP}(U)|_i = S_i + TE_{SP}(U)|_i \tag{A5}$$

using equation (A1) evaluated at i . This equation is valid only at points where U and all its derivatives are continuous. Singular points require special treatment and are excluded from the following analysis.

Define the nodal-point discretization error as the difference between the exact nodal-point solution of the approximate numerical equation and the exact solution of the exact differential equation, evaluated at i :

$$e_i = u_i - U_i \tag{A6}$$

This is the same as the node-point error defined previously. [Note that the present analysis uses a consistent definition of "error" as

$$\text{error} = \text{approximate} - \text{exact} \tag{A7}$$

Some authors sometimes use the reverse (negative) of this, which strictly should be called correction rather than error.]

Consider the discrete operator applied to the discretization error (using the assumed linearity property)

$$D(e_i) = D(u_i) - D(U_i) \tag{A8}$$

or, from equations (A2)–(A5), e_i satisfies the discrete equation

$$D(e_i) = -TE_{SP}(U)|_i = -P(U)|_i h^p + HOT \tag{A9}$$

Note that S_i from equations (A2) and (A5) has cancelled; otherwise, additional source-term errors must be retained. Now rewrite the left-hand side as

$$\begin{aligned} D(e_i) &= L(e)|_i + [D(e_i) - L(e)|_i] \\ &= L(e)|_i + TE_{SP}(e)|_i \end{aligned} \tag{A10}$$

where $e(x)$ is a continuous function, with $e_i = e(x_i)$. This means that $e(x)$ satisfies the differential equation

$$L(e)|_{i_x} = -TE_{SP}(U)|_{i_x} - TE_{SP}(e)|_{i_x} \tag{A11}$$

where i_x is the nodal value of a fixed point, $x = \text{constant}$, as h is varied. Assume that, to leading order,

$$e = O(h^q) \tag{A12}$$

where $q \geq 1$. Then equation (A11) becomes

$$\begin{aligned} L(e)|_{i_x} &= -P(U)|_{i_x} h^p + HOT + O(h^{p+q}) \\ &= O(h^p) \end{aligned} \tag{A13}$$

Since L is a linear homogeneous operator, independent of h , this also means that the leading single-point discretization error is

$$e_{i_x}^{SP} = O(h^p) \tag{A14}$$

i.e., that $q = p$. The discretization error of a discrete operator in a single-point formulation is thus of the same order as the single-point truncation error.

Finite-volume formulation

Assume that the exact differential operator given by equation (A1) is averaged over a finite-volume cell, i . The corresponding (exact) finite-volume equation is then

$$\bar{L}(U) = \bar{S}(x) \tag{A15}$$

where, in general, the operator average is

$$\bar{L} = \frac{1}{\text{VOL}} \int \int \int L \, d\bar{V} \tag{A16}$$

or, in one dimension,

$$\bar{L} = \frac{1}{h} \int_{x-h/2}^{x+h/2} L \, dx \tag{A17}$$

Again, $U(x)$ is considered to be the exact solution of the exact finite-volume equation, where $\bar{S}(x)$ is the known cell-average source term.

Let the corresponding approximate numerical finite-volume difference equation be represented by

$$D(u_i) = \bar{S}_i \tag{A18}$$

where u_i is the exact nodal-value solution of this approximate equation, and \bar{S}_i is the known exact cell-average

source term at cell i . Note that finite-volume (or, for that matter, single-point) formulations can be written in terms of cell-average values, \bar{u}_i , rather than nodal values, u_i . In general, this will involve a different discrete operator. The present analysis will focus on nodal values, but entirely similar conclusions can be reached using cell-average values.

Once again, the truncation error of the discrete finite-volume operator is defined as the difference between approximate and exact operators, operating on a test-function, v , at cell i :

$$TE_{FV}(v)|_i = D(v)|_i - \bar{L}(v)|_i \tag{A19}$$

Taylor series analysis leads to

$$TE_{FV}(v)|_i = R(v)|_i h^r + HOT \tag{A20}$$

analogous to equation (4). Using U instead of v gives

$$D(U)|_i = \bar{L}(U)|_i + TE_{FV}(U)|_i = \bar{S}_i + TE_{FV}(U)|_i \tag{A21}$$

for each cell, i .

The nodal-point discretization error is again defined by equation (A6). This now satisfies the following discrete equation

$$D(e_i) = -TE_{FV}(U)|_i = -R(U)|_i h^r + HOT \tag{A22}$$

Using equation (A10) results in a differential equation for e :

$$L(e)|_{i_x} = -TE_{FV}(U)|_{i_x} - TE_{SP}(e)|_{i_x} \tag{A23}$$

Note that the left-hand side has been written in terms of L rather than \bar{L} , since \bar{L} depends on h . Assume that, to leading order,

$$e = O(h^r) \tag{A24}$$

Then equation (A23) becomes

$$L(e)|_{i_x} = -R(U)|_{i_x} h^r + HOT + O(h^{r+p}) = O(h^r) \tag{A25}$$

as assumed, since $p \geq 2$, according to equation (12). The discretization error of a discrete operator in a finite-volume formulation is thus of the same order as the finite-volume truncation error:

$$e_{i_x}^{FV} = O(h^r) \tag{A26}$$

Note, however, that for a given discrete operator, treated alternatively as a single-point or a finite-volume operator, the corresponding respective truncation (and, hence, discretization) errors will be different. In fact, according to equation (12), they will differ by $O(h^2)$.

Finally, it should be clear that for any two different discrete operators or different (SP or FV) formulations representing a physical quantity (e.g., convection) the ratio of the discretization errors will be in the same proportion as the ratio of the respective truncation errors, as $h \rightarrow 0$. This will be demonstrated in the following section.

Examples

The model convection-diffusion problem introduced earlier forms of a good example for studying the relationship between truncation error and discretization error. For convenience, the governing equations are repeated here; written in terms of the exact solution, $U(x)$.

Single-point formulation

$$\frac{dU}{dx} - \frac{1}{Pé} \frac{d^2U}{dx^2} = 0 \tag{A27}$$

Finite-volume formulation

$$\left(\frac{U_r - U_l}{h} \right) - \frac{1}{Pé} \left(\frac{U'_r - U'_l}{h} \right) = 0 \tag{A28}$$

Boundary conditions

$$U(0) = 0 \quad U(1) = 1 \tag{A29}$$

Exact solution

$$U(x) = \frac{e^{Péx} - 1}{e^{Pé} - 1} \tag{A30}$$

Derivatives

$$\frac{dU}{dx} = \frac{Pé e^{Péx}}{e^{Pé} - 1} \quad \frac{d^2U}{dx^2} = \frac{Pé^2 e^{Péx}}{e^{Pé} - 1}, \dots \tag{A31}$$

Fundamental FV-SP relationship

$$\begin{aligned} \frac{\phi_r^{(n)} - \phi_l^{(n)}}{h} &= \phi_i^{(n+1)} + \frac{h^2}{2^2 3!} \phi_i^{(n+3)} + \frac{h^4}{2^4 5!} \phi_i^{(n+5)} \\ &+ \frac{h^6}{2^6 7!} \phi_i^{(n+7)} + \dots \end{aligned} \tag{A32}$$

Convection operators

The single-point upwind difference scheme for convection recommended in Ref. 4 can be written as

$$[SPUDS] = \frac{2\phi_{i+1} + 3\phi_i - 6\phi_{i-1} + \phi_{i-2}}{6h} \tag{A33}$$

In terms of a test-function, v , this has a Taylor expansion about grid-point i as follows

$$\begin{aligned} [SPUDS] &= \left(\frac{dv}{dx} \right)_i + \frac{v_i^{(iv)}}{12} h^3 - \frac{v_i^{(v)}}{30} h^4 + \frac{v_i^{(vi)}}{72} h^5 \\ &- \frac{v_i^{(vii)}}{252} h^6 + \dots \end{aligned} \tag{A34}$$

This is the appropriate form for a single-point formulation. Using equation (A32), for $n = 0$, gives the corresponding finite-volume formulation

$$\begin{aligned}
 [\text{SPUDS}] = & \left(\frac{v_r - v_l}{h} \right) - \frac{v_l'''}{24} h^2 + \frac{v_l^{(iv)}}{12} h^3 \\
 & - \frac{13v_l^{(v)}}{384} h^4 + \frac{v_l^{(vi)}}{72} h^5 - \frac{61v_l^{(vii)}}{15360} h^6 \\
 & + \dots \tag{A35}
 \end{aligned}$$

The QUICK convection operator can be obtained from equations (40) and (41) as

$$\begin{aligned}
 [\text{QUICK}(C)] &= \frac{\phi_r^{\text{QUICK}} - \phi_l^{\text{QUICK}}}{h} \\
 &= \frac{3\phi_{i+1} + 3\phi_i - 7\phi_{i-1} + \phi_{i-2}}{8h} \tag{A36}
 \end{aligned}$$

The Taylor expansion about grid-point i is

$$\begin{aligned}
 [\text{QUICK}(C)] &= \left(\frac{dv}{dx} \right)_i + \frac{v_l'''}{24} h^2 + \frac{v_l^{(iv)}}{16} h^3 \\
 & - \frac{11v_l^{(v)}}{480} + \frac{v_l^{(vi)}}{96} h^5 - \frac{59v_l^{(vii)}}{20160} h^6 \\
 & + \dots \tag{A37}
 \end{aligned}$$

This would be the form used in a single-point formulation. However, QUICK is specifically designed for a finite-volume formulation; using equation (A32), for $n = 0$, leads to

$$\begin{aligned}
 [\text{QUICK}(C)] &= \left(\frac{v_r - v_l}{h} \right) + \frac{v_l^{(iv)}}{16} h^3 - \frac{3v_l^{(v)}}{128} h^4 \\
 & + \frac{v_l^{(vi)}}{96} h^5 - \frac{3v_l^{(vii)}}{1024} h^6 + \dots \tag{A38}
 \end{aligned}$$

Numerical values

To get some idea of the relative size of truncation error terms, the known exact solution of the model problem is used, with $h = 1/64$. This would normally be considered a "very fine" grid; and asymptotic trends have been established, as seen in the previous tables. The truncation error for the single-point formulation of the SPUDS operator is derived from equation (A34) using U in place of v :

$$\begin{aligned}
 \text{TE}_{\text{SP}}[\text{SPUDS}] &= \frac{U_i^{(iv)}}{12} h^3 - \frac{U_i^{(v)}}{30} h^4 + \frac{U_i^{(vi)}}{72} h^5 \\
 & - \frac{U_i^{(vii)}}{252} h^6 + \dots \tag{A39}
 \end{aligned}$$

For the particular model problem being considered, this gives, at $x = 0.75$,

$$\begin{aligned}
 \text{TE}_{\text{SP}}[\text{SPUDS}] &= \left(\frac{\text{Pé}^4}{12} h^3 - \frac{\text{Pé}^5}{30} h^4 + \frac{\text{Pé}^6}{72} h^5 - \frac{\text{Pé}^7}{252} h^6 \right) \\
 & \times \left(\frac{e^{0.75\text{Pé}}}{e^{\text{Pé}} - 1} \right) \tag{A40}
 \end{aligned}$$

For $\text{Pé} = 4$ and $h = 1/64$, the numerical values of the individual terms are, respectively

$$\begin{aligned}
 \text{TE}_{\text{SP}}[\text{SPUDS}] &= (8.13802 - 0.20345 + 0.00530 \\
 & - 0.00010) \times 3.74743 \times 10^{-6} \tag{A41}
 \end{aligned}$$

or

$$\text{TE}_{\text{SP}}[\text{SPUDS}] = 2.97538 \times 10^{-5} \tag{A42}$$

Note that the second, $O(h^4)$, term in the truncation error is not insignificant.

If SPUDS is now considered (albeit inappropriately) as a finite-volume formulation, equation (A35) gives the corresponding truncation error as

$$\begin{aligned}
 \text{TE}_{\text{FV}}[\text{SPUDS}] &= -\frac{U_i'''}{24} h^2 + \frac{U_i^{(iv)}}{12} h^3 - \frac{13U_i^{(v)}}{384} h^4 \\
 & + \frac{U_i^{(vi)}}{72} h^5 - \frac{61U_i^{(vii)}}{15360} h^6 + \dots \tag{A43}
 \end{aligned}$$

with numerical values

$$\begin{aligned}
 \text{TE}_{\text{FV}}[\text{SPUDS}] &= (-65.10417 + 8.13802 - 0.20663 + 0.00530 \\
 & - 0.00002) \times 3.74743 \times 10^{-6} \tag{A44}
 \end{aligned}$$

or

$$\text{TE}_{\text{FV}}[\text{SPUDS}] = -2.14231 \times 10^{-4} \tag{A45}$$

From equation (A37), the QUICK convection scheme used (inappropriately) in a single-point formulation would have a truncation error

$$\begin{aligned}
 \text{TE}_{\text{SP}}[\text{QUICK}(C)] &= \frac{U_i'''}{24} h^2 + \frac{U_i^{(iv)}}{16} h^3 - \frac{11U_i^{(v)}}{480} h^4 + \frac{U_i^{(vi)}}{96} h^5 \\
 & - \frac{59U_i^{(vii)}}{20160} h^6 + \dots \tag{A46}
 \end{aligned}$$

giving numerical values

$$\begin{aligned}
 \text{TE}_{\text{SP}}[\text{QUICK}(C)] &= (65.10417 + 6.10352 - 0.13987 + 0.00397 \\
 & - 0.00007) \times 3.74743 \times 10^{-6} \tag{A47}
 \end{aligned}$$

or

$$\text{TE}_{\text{SP}}[\text{QUICK}(C)] = 2.66336 \times 10^{-4} \tag{A48}$$

By contrast, the (appropriate) finite-volume formulation of QUICK leads to

$$\begin{aligned} \text{TE}_{\text{FV}}[\text{QUICK}(C)] &= \frac{U_i^{(iv)}}{16}h^3 - \frac{3U_i^{(v)}}{128}h^4 \\ &+ \frac{U_i^{(vi)}}{96}h^5 - \frac{3U_i^{(vii)}}{1024}h^6 + \dots \end{aligned} \quad (\text{A49})$$

with numerical values

$$\begin{aligned} \text{TE}_{\text{FV}}[\text{QUICK}(C)] &= (6.10352 - 0.14305 + 0.00397 - 0.00007) \\ &\times 3.74743 \times 10^{-6} \end{aligned} \quad (\text{A50})$$

or

$$\text{TE}_{\text{FV}}[\text{QUICK}(C)] = 2.23511 \times 10^{-5} \quad (\text{A51})$$

Recall from Tables 1 and 2, node-point errors for $h = 1/64$:

$$\text{NPE}_{\text{FV}}[\text{QUICK}(C)] = -5.30547084 \times 10^{-6} \quad (\text{A52})$$

$$\text{NPE}_{\text{FV}}[\text{SPUDS}] = +5.08534128 \times 10^{-5} \quad (\text{A53})$$

$$\text{NPE}_{\text{SP}}[\text{SPUDS}] = -7.06282736 \times 10^{-6} \quad (\text{A54})$$

$$\text{NPE}_{\text{SP}}[\text{QUICK}(C)] = -6.32202472 \times 10^{-5} \quad (\text{A55})$$

Note, in particular, the ratio of the single-point SPUDS error to the finite-volume QUICK (C) error (i.e., the two third-order methods):

$$\frac{\text{NPE}_{\text{SP}}[\text{SPUDS}]}{\text{NPE}_{\text{FV}}[\text{QUICK}(C)]} = 1.33 \dots \quad (\text{A56})$$

This is virtually the same as the ratio of the respective leading truncation error terms. From equations (A39) and (A49),

$$\frac{\text{LTE}_{\text{SP}}[\text{SPUDS}]}{\text{LTE}_{\text{FV}}[\text{QUICK}(C)]} = \frac{4}{3} \quad (\text{A57})$$

This relationship will be found to be (approximately) true for other ratios, as well.

Diffusion operators

The second-order central-difference operator for diffusion is

$$[\text{CDS2}] = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{h^2} \quad (\text{A58})$$

This can be viewed as a single-point operator

$$\begin{aligned} [\text{CDS2}] &= \left(\frac{d^2}{dx^2} \right)_i + \frac{v_i^{(iv)}}{12}h^2 + \frac{v_i^{(vi)}}{360}h^4 + \frac{v_i^{(viii)}}{20160}h^6 \\ &+ \dots \end{aligned} \quad (\text{A59})$$

or a finite-volume operator, using equation (12), with $n = 1$,

$$\begin{aligned} [\text{CDS2}] &= \left(\frac{v'_r - v'_l}{h} \right) + \frac{v_i^{(iv)}}{24}h^2 + \frac{13v_i^{(vi)}}{5760}h^4 \\ &+ \frac{v_i^{(viii)}}{21504}h^6 + \dots \end{aligned} \quad (\text{A60})$$

Note that the latter form (with the smaller truncation error) corresponds to the QUICK finite-volume formulation of diffusion, QUICK(D).

For $\text{Pé} = 4$ and $h = 1/64$, the respective numerical values are

$$\begin{aligned} \text{TE}_{\text{SP}}[\text{CDS2}] &= (5.20833 \times 10^{-3} + 6.78168 \times 10^{-7} \\ &+ 4.73053 \times 10^{-11}) \\ &\times 3.74743 \times 10^{-1} \end{aligned} \quad (\text{A61})$$

and

$$\begin{aligned} \text{TE}_{\text{FV}}[\text{QUICK}(D)] &= (2.60417 \times 10^{-3} + 5.51012 \\ &\times 10^{-7} + 4.43487 \times 10^{-11}) \\ &\times 3.74743 \times 10^{-1} \end{aligned} \quad (\text{A62})$$

In either case, the leading term is dominant. Note that

$$\frac{\text{LTE}_{\text{SP}}[\text{CDS2}]}{\text{LTE}_{\text{FV}}[\text{QUICK}(D)]} = 2 \quad (\text{A63})$$

This is reflected in the node-point error of Table 3, where

$$\text{NPE}_{\text{FV}}[\text{QUICK}(D)] = +6.38006991 \times 10^{-5} \quad (\text{A64})$$

and

$$\text{NPE}_{\text{SP}}[\text{CDS2}] = +1.27591015 \times 10^{-4} \quad (\text{A65})$$

This means that the finite-volume (QUICK) formulation of diffusion is twice as accurate as the single-point CDS2 formulation, although both are formally second-order accurate.

The fourth-order single-point diffusion operator given by equation (16) has a single-point truncation error

$$\begin{aligned} \text{TE}_{\text{SP}}[\text{equation (16)}] &= -\frac{U_i^{(vi)}}{90}h^4 - \frac{U_i^{(viii)}}{1008}h^6 + \dots \end{aligned} \quad (\text{A66})$$

When used (inappropriately) as a finite-volume operator, this gives

$$\begin{aligned} \text{TE}_{\text{FV}}[\text{equation (16)}] &= -\frac{U_i^{(iv)}}{24}h^2 - \frac{13U_i^{(vi)}}{1152}h^4 - \frac{107U_i^{(viii)}}{107520}h^6 + \dots \end{aligned} \quad (\text{A67})$$

which, of course, is only second-order accurate, according to equation (12).

By contrast, the fourth-order finite-volume operator given by equation (17) has a finite-volume truncation error

$$TE_{FV}[\text{equation (17)}] = -\frac{3U_i^{(vi)}}{640}h^4 - \frac{193U_i^{(viii)}}{322560}h^6 + \dots \quad (A68)$$

And if this were used (inappropriately) in a single-point formulation, the truncation error would be

$$TE_{SP}[\text{equation (17)}] = \frac{U_i^{(iv)}}{24}h^2 - \frac{U_i^{(vi)}}{240}h^4 - \frac{19U_i^{(viii)}}{1080}h^6 + \dots \quad (A69)$$

again, second-order, according to equation (12). Note that

$$\frac{LTE_{SP}[\text{equation (16)}]}{LTE_{FV}[\text{equation (17)}]} = 2.37\dots \quad (A70)$$

From Tables 4 and 5, for $h = 1/64$.

$$\frac{NPE_{SP}[\text{equation (16)}]}{NPE_{FV}[\text{equation (17)}]} = \frac{-6.59600528 \times 10^{-8}}{-2.79314528 \times 10^{-8}} = 2.36\dots \quad (A71)$$

Again, one sees that the finite-volume fourth-order formulation is significantly more accurate than the single-point fourth-order formulation.

Convection-diffusion operators

The standard QUICK scheme for both convection and diffusion can be written

$$[\text{QUICK}] = \left(\frac{3\phi_{i+1} + 3\phi_i - 7\phi_{i-1} + \phi_{i-2}}{8h} \right) - \frac{1}{P\acute{e}} \left(\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{h^2} \right) \quad (A72)$$

Viewed as a finite-volume formulation, this gives

$$[\text{QUICK}] = \left(\frac{v_r - v_l}{h} \right) - \frac{1}{P\acute{e}} \left(\frac{v'_r - v'_l}{h} \right) - \frac{1}{P\acute{e}} \left(\frac{v_i^{(iv)}}{24} \right) h^2 + \left(\frac{v_i^{(iv)}}{16} \right) h^3 - \left[\frac{3}{128} v_i^{(v)} + \frac{1}{P\acute{e}} \left(\frac{13v_i^{(vi)}}{5760} \right) \right] h^4 + \left(\frac{v_i^{(vi)}}{96} \right) h^5 - \left[\frac{3v_i^{(vii)}}{1024} + \frac{1}{P\acute{e}} \left(\frac{v_i^{(viii)}}{21504} \right) \right] h^6 + \dots \quad (A73)$$

Whereas a single-point analysis would give

$$[\text{QUICK}] = \left(\frac{dv}{dx} \right)_i - \frac{1}{P\acute{e}} \left(\frac{d^2v}{dx^2} \right)_i + \left(\frac{v_i'''}{24} - \frac{1}{P\acute{e}} \frac{v_i^{(iv)}}{12} \right) h^2 + \left(\frac{v_i^{(iv)}}{16} \right) h^3 - \left[\frac{11v_i^{(v)}}{480} + \frac{1}{P\acute{e}} \left(\frac{v_i^{(vi)}}{360} \right) \right] h^4 + \left(\frac{v_i^{(vi)}}{96} \right) h^5 - \left[\frac{59v_i^{(vii)}}{20160} + \frac{1}{P\acute{e}} \left(\frac{v_i^{(viii)}}{20160} \right) \right] h^6 + \dots \quad (A74)$$

Although the truncation error terms look different, it is not hard to show that, in fact, in terms of U , they are identical. For example, since U satisfies the exact equation

$$\frac{dU}{dx} = \frac{1}{P\acute{e}} \frac{d^2U}{dx^2} \quad (A75)$$

then

$$U''' = \frac{1}{P\acute{e}} U^{(iv)} \quad (A76)$$

and the leading single-point truncation error term becomes

$$\left(\frac{U_i'''}{24} - \frac{1}{P\acute{e}} \frac{U_i^{(iv)}}{12} \right) h^2 = \left(\frac{1}{P\acute{e}} \frac{U_i^{(iv)}}{24} - \frac{1}{P\acute{e}} \frac{U_i^{(iv)}}{12} \right) h^2 = -\frac{1}{P\acute{e}} \left(\frac{U_i^{(iv)}}{12} \right) h^2 \quad (A77)$$

and, similarly for the other terms.

The SPUDS-plus-CDS2 convection-diffusion scheme can be written as

$$[\text{SPUDS} + \text{CDS2}] = \left(\frac{2\phi_{i+1} + 3\phi_i - 6\phi_{i-1} + \phi_{i-2}}{6h} \right) - \frac{1}{P\acute{e}} \left(\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{h^2} \right) \quad (A78)$$

As a single-point formulation, this gives

$$[\text{SPUDS} + \text{CDS2}] = \left(\frac{dv}{dx} \right)_i - \frac{1}{P\acute{e}} \left(\frac{d^2v}{dx^2} \right)_i - \frac{1}{P\acute{e}} \left(\frac{v_i^{(iv)}}{12} \right) h^2 + \left(\frac{v_i^{(iv)}}{12} \right) h^3 - \left[\frac{v_i^{(v)}}{30} + \frac{1}{P\acute{e}} \left(\frac{v_i^{(vi)}}{360} \right) \right] h^4 + \left(\frac{v_i^{(vi)}}{72} \right) h^5 - \left[\frac{v_i^{(vii)}}{252} + \frac{1}{P\acute{e}} \left(\frac{v_i^{(viii)}}{20160} \right) \right] h^6 + \dots \quad (A79)$$

whereas, for a finite-volume formulation,

$$\begin{aligned}
 & [\text{SPUDS} + \text{CDS2}] \\
 &= \left(\frac{v_r - v_l}{h} \right) - \frac{1}{\text{Pé}} \left(\frac{v'_r - v'_l}{h} \right) \\
 &\quad - \left[\frac{v_i'''}{24} + \frac{1}{\text{Pé}} \left(\frac{v_i^{(iv)}}{24} \right) \right] h^2 + \left(\frac{v_i^{(iv)}}{12} \right) h^3 \\
 &\quad - \left[\frac{13v_i^{(v)}}{384} + \frac{1}{\text{Pé}} \left(\frac{13v_i^{(vi)}}{5760} \right) \right] h^4 + \left(\frac{v_i^{(vi)}}{72} \right) h^5 \\
 &\quad - \left[\frac{61v_i^{(vii)}}{1530} + \frac{1}{\text{Pé}} \left(\frac{v_i^{(viii)}}{21504} \right) \right] h^6 + \dots \quad (\text{A80})
 \end{aligned}$$

Once again, in terms of U , the two truncation errors are identical.

Note that, because of the dominance of the second-order diffusion terms, as $h \rightarrow 0$,

$$\frac{\text{LTE}[\text{SPUDS} + \text{CDS2}]}{\text{LTE}[\text{QUICK}]} = 2 \quad (\text{A81})$$

This is borne out in *Table 6*, where it is seen that, for $h = 1/64$,

$$\begin{aligned}
 \frac{\text{NPE}[\text{SPUDS} + \text{CDS2}]}{\text{NPE}[\text{QUICK}]} &= \frac{9.97187451 \times 10^{-5}}{4.82503616 \times 10^{-5}} \\
 &= 2.07 \quad (\text{A82})
 \end{aligned}$$

Finally, it should be noted that in high-convection problems, where the grid Péclet number

$$P_\Delta = h \text{Pé} \quad (\text{A83})$$

is large, the appropriate way to write the leading truncation error terms is as follows:

$$\text{LTE}_{\text{FV}}[\text{QUICK}] = \frac{U_i^{(iv)}}{16} \left(1 - \frac{2}{3P_\Delta} \right) h^3 \quad (\text{A84})$$

and

$$\text{LTE}_{\text{SP}}[\text{SPUDS} + \text{CDS2}] = \frac{U_i^{(iv)}}{12} \left(1 - \frac{1}{P_\Delta} \right) h^3 \quad (\text{A85})$$

This means that, for most flows of interest, using practical grids (so that P_Δ is very large), these convection-diffusion schemes are effectively third-order accurate (even though only formally second-order accurate as $h \rightarrow 0$).

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