Comparison of truncation error of finite-difference and finite-volume formulations of convection terms

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This paper explains significant differences in spatial truncation error between formulations of convection involving a finite-difference approximation of the first derivative, on the one hand, and a finite-volume model of flux differences across a control volume cell on the other. The difference between the two formulations involves a second-order truncation error term (proportional to the third derivative of the convected variable). Hence, for example, a third- (or higher) order finite-difference approximation for the first-derivative convection term is only second-order accurate when written in conservative control volume form as a finite-volume formulation, and vice versa.

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

Finite-difference and finite-volume formulations

Consider the model constant-coefficient one-dimensional pure convection equation for a scalar ϕ

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = S(x, t) \tag{1}$$

where S is a known source term, and assume that a numerical solution is sought using a discrete grid of constant step width h. As usual, let ϕ_i represent the numerical approximation of ϕ at grid point i.

A finite-difference formulation of equation (1) attempts to simulate

$$\frac{\partial \phi_i}{\partial t} = -u\left(\frac{\partial \phi}{\partial x}\right)_i + S_i(t) \tag{2}$$

and, in particular, the spatial first-derivative convection term is written in terms of node values of ϕ. The *modelled* first derivative is then equal to the true first derivative at i, plus truncation error terms:

$$\left(\frac{\partial \phi}{\partial x}\right)_{\text{model}} = \left(\frac{\partial \phi}{\partial x}\right)_i + (\text{TE})_{\text{FD}} \tag{3}$$

The leading term in $(\text{TE})_{\text{FD}}$ (i.e., the term involving the *lowest* power of h) is conventionally called the "order" of the finite-difference discretization.

On the other hand, consider integrating equation (2) with respect to x, from $-h/2$ to $+h/2$, and dividing by h. This gives

$$\frac{\partial \bar{\phi}_i}{\partial t} = -\frac{u(\phi_r - \phi_l)}{h} + \bar{S}_i(t) \tag{4}$$

where the bars refer to spatial averages, and left and right control volume face values are indicated. This is the finite-volume formulation of equation (1). In this case, one writes

$$\frac{(\phi_r - \phi_l)_{\text{model}}}{h} = \frac{(\phi_r - \phi_l)}{h} + (\text{TE})_{\text{FV}} \tag{5}$$

where the right-hand side involves the true face value difference. Once again, the leading term in $(\text{TE})_{\text{FV}}$ is the order of the finite-volume discretization.

It is often assumed (especially in recent CFD literature) that, if a finite-difference model is written in flux difference form, then $(\text{TE})_{\text{FD}}$ is the same as $(\text{TE})_{\text{FV}}$. But, as will be shown, except for the leading term in first-order formulations,

$$(\text{TE})_{\text{FD}} \neq (\text{TE})_{\text{FV}} \tag{6}$$

The confusion is apparently based on the fact that the finite-difference model of the first derivative can often be split into two parts, i.e.,

$$\left(\frac{\partial \phi}{\partial x}\right)_{\text{model}} = \frac{\phi_r^* - \phi_l^*}{h} \tag{7}$$

where $\phi_l^*(i) = \phi_r^*(i-1)$, and this is sometimes treated as a finite-volume formulation (with the assumption that the truncation error is the same). But if equation (7) is

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to be treated as a finite-volume model, one must *recompute* the truncation error according to equation (5).

Face-centered Taylor expansions

For definiteness, consider the classical second-order central finite-difference approximation for the first derivative:

$$\left(\frac{\partial \phi}{\partial x}\right)_{\text{model}} = \frac{\phi_{i+1} - \phi_{i-1}}{2h} \tag{8}$$

First, make Taylor expansions about grid point i. For example,

$$\phi_{i+1} = \phi_i + \phi_i' h + \tfrac{1}{2}\phi_i'' h^2 + \tfrac{1}{6}\phi_i''' h^3 + \cdots \tag{9}$$

and

$$\phi_{i-1} = \phi_i - \phi_i' h + \tfrac{1}{2}\phi_i'' h^2 - \tfrac{1}{6}\phi_i''' h^3 + \cdots \tag{10}$$

so that

$$\phi_{i+1} - \phi_{i-1} = 2\phi_i' h + \tfrac{1}{3}\phi_i''' h^3 + \tfrac{1}{60}\phi_i^{(v)} h^5 + \cdots \tag{11}$$

thus giving the well-known result that

$$\frac{\phi_{i+1} - \phi_{i-1}}{2h} = \left(\frac{\partial \phi}{\partial x}\right)_i + \frac{1}{6}\phi_i''' h^2 + \frac{1}{120}\phi_i^{(v)} h^4 + \cdots \tag{12}$$

verifying that this is, indeed, a second-order approximation to the first derivative. But this model can be rewritten in the form of equation (7) by identifying

$$\phi_r^* = \frac{\phi_{i+1} + \phi_i}{2} \tag{13}$$

and

$$\phi_l^* = \frac{\phi_i + \phi_{i-1}}{2} \tag{14}$$

In other words, the modelled left and right face values are taken to be just the arithmetic means of the node values on adjacent sides of the individual faces. Note, as required by conservation, that

$$\phi_l^*(i) = \phi_r^*(i-1) \tag{15}$$

Now the model can be considered as a finite-volume formulation simply by writing

$$\frac{\phi_r^* - \phi_l^*}{h} = \frac{\left(\frac{\phi_{i+1} + \phi_i}{2}\right) - \left(\frac{\phi_i + \phi_{i-1}}{2}\right)}{h} = \frac{(\phi_r - \phi_l)}{h} + (\text{TE})_{\text{FV}} \tag{16}$$

In order to assess the truncation error, expand the node values about individual control volume *face* locations:

$$\phi_{i+1} = \phi_r + \phi_r'\left(\frac{h}{2}\right) + \frac{1}{2}\phi_r''\left(\frac{h}{2}\right)^2 + \frac{1}{6}\phi_r'''\left(\frac{h}{2}\right)^3 + \cdots \tag{17}$$

$$\phi_i = \phi_r - \phi_r'\left(\frac{h}{2}\right) + \frac{1}{2}\phi_r''\left(\frac{h}{2}\right)^2 - \frac{1}{6}\phi_r'''\left(\frac{h}{2}\right)^3 + \cdots \tag{18}$$

$$\phi_i = \phi_l + \phi_l'\left(\frac{h}{2}\right) + \frac{1}{2}\phi_l''\left(\frac{h}{2}\right)^2 + \frac{1}{6}\phi_l'''\left(\frac{h}{2}\right)^3 + \cdots \tag{19}$$

$$\phi_{i-1} = \phi_l - \phi_l'\left(\frac{h}{2}\right) + \frac{1}{2}\phi_l''\left(\frac{h}{2}\right)^2 - \frac{1}{6}\phi_l'''\left(\frac{h}{2}\right)^3 + \cdots \tag{20}$$

Then the individual modelled face values are given by

$$\phi_r^* = \frac{\phi_{i+1} + \phi_i}{2} = \phi_r + \frac{1}{8}\phi_r'' h^2 + \frac{1}{384}\phi_r^{(iv)} h^4 + \cdots \tag{21}$$

and

$$\phi_l^* = \frac{\phi_i + \phi_{i-1}}{2} = \phi_l + \frac{1}{8}\phi_l'' h^2 + \frac{1}{384}\phi_l^{(iv)} h^4 + \cdots \tag{22}$$

so that

$$\frac{(\phi_r^* - \phi_l^*)}{h} = \frac{(\phi_r - \phi_l)}{h} + \frac{1}{8}\left(\frac{\phi_r'' - \phi_l''}{h}\right)h^2 + \frac{1}{384}\left(\frac{\phi_r^{(iv)} - \phi_l^{(iv)}}{h}\right)h^4 \cdots \tag{23}$$

But, from Equations (17) and (18),

$$\phi_r'' = 4\left(\frac{\phi_{i+1} - 2\phi_r + \phi_i}{h^2}\right) + \cdots \tag{24}$$

and similarly for ϕ_l''. Then, using equation (9) together with the following expansions of face values about grid point i,

$$\phi_r = \phi_i + \phi_i'\left(\frac{h}{2}\right) + \frac{1}{2}\phi_i''\left(\frac{h}{2}\right)^2 + \frac{1}{6}\phi_i'''\left(\frac{h}{2}\right)^3 + \cdots \tag{25}$$

and

$$\phi_l = \phi_i - \phi_i'\left(\frac{h}{2}\right) + \frac{1}{2}\phi_i''\left(\frac{h}{2}\right)^2 - \frac{1}{6}\phi_i'''\left(\frac{h}{2}\right)^3 + \cdots \tag{26}$$

the difference of face second derivatives appearing in equation (23) can be written as

$$\frac{\phi_r'' - \phi_l''}{h} = \phi_i''' + \frac{1}{24}\phi_i^{(v)} h^2 + \frac{1}{1920}\phi_i^{(vii)} h^4 + \cdots \tag{27}$$

giving

$$\frac{\left(\frac{\phi_{i+1} + \phi_i}{2}\right) - \left(\frac{\phi_i + \phi_{i-1}}{2}\right)}{h} = \frac{(\phi_r - \phi_l)}{h} + \frac{1}{8}\phi_i''' h^2 + \frac{1}{128}\phi_i^{(v)} h^4 + \cdots \tag{28}$$

Thus, by comparing equations (12) and (28), one sees that

$$(\text{TE})_{\text{FD}} = \tfrac{1}{6}\phi_i'''h^2 + \tfrac{1}{120}\phi_i^{(v)}h^4 + \cdots \quad (29)$$

whereas

$$(\text{TE})_{\text{FV}} = \tfrac{1}{8}\phi_i'''h^2 + \tfrac{1}{128}\phi_i^{(v)}h^4 + \cdots \quad (30)$$

This, of course, is a significant difference, even though both formulations are second-order accurate. Note that the difference in the truncation errors is

$$(\text{TE})_{\text{FD}} - (\text{TE})_{\text{FV}} = \tfrac{1}{24}\phi_i'''h^2 + \tfrac{1}{1920}\phi_i^{(v)}h^4 + \cdots \quad (31)$$

and a result similar to this will be found in general to be true for any convection formula that can be simultaneously viewed either as a finite-difference formula for $(\partial\phi/\partial x)_i$ or a finite-volume formula for $(\phi_r - \phi_l)/h$. In fact, referring to equations (25) and (26), continued through fifth-order, one finds that, irrespective of the numerical scheme,

$$\frac{(\phi_r - \phi_l)}{h} = \left(\frac{\partial\phi}{\partial x}\right)_i + \frac{1}{24}\phi_i'''h^2 + \frac{1}{1920}\phi_i^{(v)}h^4 + \cdots \quad (32)$$

which explains the difference between equations (29) and (30).

Other common discretizations

In addition to the second-order central-difference formulation considered above, it is convenient to summarize a number of other discretizations commonly used in convective modelling.

First-order upwinding

For $u > 0$, the convective term in equation (2) is written

$$-u\left(\frac{\partial\phi}{\partial x}\right) = -u\left(\frac{\phi_i - \phi_{i-1}}{h}\right) \quad (33)$$

From equation (10), viewed as a finite-difference formulation, this gives

$$\frac{(\phi_i - \phi_{i-1})}{h} = \left(\frac{\partial\phi}{\partial x}\right)_i - \frac{1}{2}\phi_i''h + \frac{1}{6}\phi_i'''h^2 - \cdots \quad (34)$$

which, as expected, is first-order accurate. Viewed as a finite-volume model, for $u > 0$, the face values are written (with upwind bias) as

$$(\phi_r)_{\text{model}} = \phi_i = \phi_r - \phi_r'\left(\frac{h}{2}\right) + \cdots \quad (35)$$

and

$$(\phi_l)_{\text{model}} = \phi_{i-1} = \phi_l - \phi_l'\left(\frac{h}{2}\right) + \cdots \quad (36)$$

And this gives

$$\frac{(\phi_r - \phi_l)_{\text{model}}}{h} = \frac{(\phi_r - \phi_l)}{h} - \frac{1}{2}\left(\frac{\phi_r' - \phi_l'}{h}\right)h + \cdots \quad (37)$$

But, from equations (17)–(20),

$$\phi_r' = \frac{(\phi_{i+1} - \phi_i)}{h} - \frac{1}{24}\phi_r'''h^2 + \cdots \quad (38)$$

and

$$\phi_l' = \frac{(\phi_i - \phi_{i-1})}{h} - \frac{1}{24}\phi_l'''h^2 + \cdots \quad (39)$$

so that

$$\frac{\phi_r' - \phi_l'}{h} = \frac{(\phi_{i+1} - 2\phi_i + \phi_{i-1})}{h^2} - \frac{1}{24}\frac{(\phi_r''' - \phi_l''')}{h}h^2 + \cdots \quad (40)$$

and the second central-difference can be written

$$\frac{(\phi_{i+1} - 2\phi_i + \phi_{i-1})}{h^2} = \phi_i'' + \frac{1}{12}\phi_i^{(iv)}h^2 + \cdots \quad (41)$$

as is well known. This means that equation (37) becomes

$$\frac{(\phi_r - \phi_l)_{\text{model}}}{h} = \frac{(\phi_r - \phi_l)}{h} - \frac{1}{2}\phi_i''h + \cdots \quad (42)$$

so that the *leading* truncation error is the same as that of the finite-difference formula, equation (34). This, of course, is to be expected from equation (32).

Second-order upwinding

For $u > 0$, if one interpolates a fully upwind-biased parabola through i, $(i-1)$, and $(i-2)$, the corresponding first derivative at i is

$$\left(\frac{\partial\phi}{\partial x}\right)_{\text{model}} = \frac{(3\phi_i - 4\phi_{i-1} + \phi_{i-2})}{2h} \quad (43)$$

$$= \left(\frac{\partial\phi}{\partial x}\right)_i - \frac{1}{3}\phi_i'''h^2 + \frac{1}{4}\phi_i^{(iv)}h^3 + \cdots \quad (44)$$

But the right-hand side of equation (43) can also be written in finite-volume form as

$$\frac{(\tfrac{3}{2}\phi_i - \tfrac{1}{2}\phi_{i-1}) - (\tfrac{3}{2}\phi_{i-1} - \tfrac{1}{2}\phi_{i-2})}{h} = \frac{(\phi_r - \phi_l)}{h} - \frac{3}{8}\phi_i'''h^2 - \frac{1}{4}\phi_i^{(iv)}h^3 + \cdots \quad (45)$$

which again conforms with equation (32). Note that, in this case, face values are obtained by linear *extrapolation* from upwind nodes.

Third-order upwinding

This time, for $u > 0$, interpolate a (partially upwinded) cubic through $(i+1)$, i, $(i-1)$, and $(i-2)$. The corresponding first derivative at i is then

$$\left(\frac{\partial\phi}{\partial x}\right)_{\text{model}} = \frac{(\phi_{i+1} - \phi_{i-1})}{2h} - \frac{(\phi_{i+1} - 3\phi_i + 3\phi_{i-1} - \phi_{i-2})}{6h} \tag{46}$$

Written in this form, one can see that the third difference will cancel the leading truncation error in equation (12), giving

$$\left(\frac{\partial\phi}{\partial x}\right)_{\text{model}} = \left(\frac{\partial\phi}{\partial x}\right)_i + \frac{1}{12}\phi_i^{(\text{iv})}h^3 - \frac{1}{30}\phi_i^{(\text{v})}h^4 + \cdots \tag{47}$$

which is indeed a third-order accurate representation of the first derivative at i. On the other hand, equation (46) can be rewritten in finite-volume form by identifying face values (for $u > 0$) as

$$(\phi_r)_{\text{model}} = \frac{(\phi_{i+1} + \phi_i)}{2} - \frac{1}{6}(\phi_{i+1} - 2\phi_i + \phi_{i-1}) \tag{48}$$

and

$$(\phi_l)_{\text{model}} = \frac{(\phi_i + \phi_{i-1})}{2} - \frac{1}{6}(\phi_i - 2\phi_{i-1} + \phi_{i-2}) \tag{49}$$

But this gives

$$\frac{(\phi_r - \phi_l)_{\text{model}}}{h} = \frac{(\phi_r - \phi_l)}{h} - \frac{1}{24}\phi_i'''h^2 + \frac{1}{12}\phi_i^{(\text{iv})}h^3 + \cdots \tag{50}$$

which of course is only a second-order accurate approximation.

To achieve a third-order accurate finite-volume representation, one needs to annihilate the leading truncation error in equation (28). This is achieved by writing (for $u > 0$)

$$(\phi_r)_{\text{model}} = \frac{(\phi_{i+1} + \phi_i)}{2} - \frac{1}{8}(\phi_{i+1} - 2\phi_i + \phi_{i-1}) \tag{51}$$

and

$$(\phi_l)_{\text{model}} = \frac{(\phi_i + \phi_{i-1})}{2} - \frac{1}{8}(\phi_i - 2\phi_{i-1} + \phi_{i-2}) \tag{52}$$

giving

$$\frac{(\phi_r - \phi_l)_{\text{model}}}{h} = \frac{\phi_r - \phi_l}{h} + \frac{1}{16}\phi_i^{(\text{iv})}h^3 - \frac{3}{128}\phi_i^{(\text{v})}h^4 + \cdots \tag{53}$$

which is seen to be third-order accurate. Equations (51) and (52) represent the well-known QUICK formulas for face values, obtained by interpolating a parabola through the two nearest node values together with that of the next adjacent upwind node. In summary, the 1/8 factor on the second-difference terms is appropriate for a finite-volume formulation, whereas the 1/6 factor corresponds to the finite-difference model of the derivative. In practice, the difference between using 1/8 and 1/6 (in a finite-volume formulation) is observed to be quite small. Note that second-order upwinding can also be written in a similar form, using a factor of 1/2 on the second-difference terms. In this case, however, results are significantly less accurate.

Higher-order formulations

The simplest way to construct higher-order formulas is to start with a known formula and add higher-order difference terms to cancel the leading truncation error. For example, if one were trying to construct a fourth-order accurate approximation to the first derivative at i, the appropriate formula would cancel the ϕ_i''' term in equation (12) without introducing an h^3 term. This can be done by using the *average* third difference centered at node i given by

$$\begin{aligned}\tfrac{1}{2}[(\phi_{i+2} - 3\phi_{i+1} + 3\phi_i - \phi_{i-1}) \\ + (\phi_{i+1} - 3\phi_i + 3\phi_{i-1} - \phi_{i-2})] \\ = \tfrac{1}{2}(\phi_{i+2} - 2\phi_{i+1} + 2\phi_{i-1} - \phi_{i-2})\end{aligned} \tag{54}$$

so that

$$\left(\frac{\partial\phi}{\partial x}\right)_{\text{model}} = \frac{(\phi_{i+1} - \phi_{i-1})}{2h} - \frac{(\phi_{i+2} - 2\phi_{i+1} + 2\phi_{i-1} - \phi_{i-2})}{12h} \tag{55}$$

On the other hand, the appropriate fourth-order finite-volume formulation would use the *average* second difference centered at a face. For example,

$$\begin{aligned}\tfrac{1}{2}[(\phi_{i+2} - 2\phi_{i+1} + \phi_i) + (\phi_{i+1} - 2\phi_i + \phi_{i-1})] \\ = \tfrac{1}{2}(\phi_{i+2} - \phi_{i+1} - \phi_i + \phi_{i-1})\end{aligned} \tag{56}$$

so that the appropriate face value is

$$(\phi_r)_{\text{model}} = \frac{(\phi_{i+1} + \phi_i)}{2} - \frac{(\phi_{i+2} - \phi_{i+1} - \phi_i + \phi_{i-1})}{16} \tag{57}$$

with a similar formula for ϕ_l (reducing all indexes by 1).

Once again, one sees that equation (55) could be rewritten in finite-volume form using

$$(\phi_r)_{\text{model}} = \frac{(\phi_{i+1} + \phi_i)}{2} - \frac{(\phi_{i+2} - \phi_{i+1} - \phi_i + \phi_{i-1})}{12} \tag{58}$$

with a similar formula for the left face. But this would result in a finite-volume formulation that is only *second*-order accurate, as predicted by equation (32).

Conclusion

Equation (32) shows that there is a significant difference between the first derivative at a node and the face value difference (divided by h) across a control volume cell. If a convection scheme is constructed on the basis of modelling $(\partial\phi/\partial x)_i$, with truncation error $(\mathrm{TE})_{\mathrm{FD}}$, and then rewritten in conservative finite-volume form, the truncation error must be recomputed according to equation (5), using Taylor expansions about *face* values. The difference in accuracy shows up in *steady-state* calculations, where $\partial\phi_i/\partial t = \partial\bar{\phi}_i/\partial t = 0$. Interestingly enough, if one writes, in the vicinity of grid point i,

$$\phi(x) = \phi_i + \phi_i' x + \tfrac{1}{2}\phi_i'' x^2 + \tfrac{1}{6}\phi_i''' x^3 + \tfrac{1}{24}\phi_i^{(\mathrm{iv})} x^4 + \cdots \tag{59}$$

and then computes the control volume cell average

$$\bar{\phi}_i = \frac{1}{h}\int_{-h/2}^{h/2} \phi(x)\,dx \tag{60}$$

the result is

$$\bar{\phi}_i = \phi_i + \tfrac{1}{24}\phi_i'' h^2 + \tfrac{1}{1920}\phi_i^{(\mathrm{iv})} h^4 + \cdots \tag{61}$$

This, for example, explains the difference between the 1/8 factor in the third-order *steady-state* QUICK scheme and the 1/6 factor in the third-order *time-accurate* QUICKEST scheme, which was pointed out 15 years ago.[1]

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Reference

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