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Comparison of Truncation Error of Finite-Difference and Finite-Volume Formulations of Convection Terms

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COMPARISON OF TRUNCATION ERROR OF FINITE-DIFFERENCE AND FINITE-VOLUME FORMULATIONS OF CONVECTION TERMS

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SUMMARY

Judging by errors in the computational-fluid-dynamics literature in recent years, it is not generally well understood that (above first-order) there are 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*.

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.

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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:

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

The leading term in $(\text{T.E.})_{\text{FD}}$ (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

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

where the right-hand side involves the true face-value difference. Once again, the leading term in $(\text{T.E.})_{\text{FV}}$ 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 $(\text{T.E.})_{\text{FD}}$ is the same as $(\text{T.E.})_{\text{FV}}$. But, as will be shown, except for the leading term in first-order formulations,

$$(\text{T.E.})_{\text{FD}} \neq (\text{T.E.})_{\text{FV}} \tag{6}$$

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.,

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

where $\phi_\ell^*(i) = \phi_r^*(i-1)$, 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 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,

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

and

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

so that

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

thus giving the well-known result that

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

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

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

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

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

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

$$\frac{\phi_r^* - \phi_\ell^*}{h} = \frac{\left(\dfrac{\phi_{i+1} + \phi_i}{2}\right) - \left(\dfrac{\phi_i + \phi_{i-1}}{2}\right)}{h} = \frac{(\phi_r - \phi_\ell)}{h} + (\text{T.E.})_{\text{FV}} \tag{16}$$

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

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

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

$$\phi_i = \phi_\ell + \phi_\ell'\left(\frac{h}{2}\right) + \tfrac{1}{2}\,\phi_\ell''\left(\frac{h}{2}\right)^2 + \tfrac{1}{6}\,\phi_\ell'''\left(\frac{h}{2}\right)^3 + \ldots \tag{19}$$

$$\phi_{i-1} = \phi_\ell - \phi_\ell'\left(\frac{h}{2}\right) + \tfrac{1}{2}\,\phi_\ell''\left(\frac{h}{2}\right)^2 - \tfrac{1}{6}\,\phi_\ell'''\left(\frac{h}{2}\right)^3 + \ldots \tag{20}$$

Then the individual modelled face-values are given by

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

and

$$\phi_\ell^* = \frac{\phi_i + \phi_{i-1}}{2} = \phi_\ell + \tfrac{1}{8}\,\phi_\ell''\,h^2 + \tfrac{1}{384}\,\phi_\ell^{(\mathrm{iv})}\,h^4 + \ldots \tag{22}$$

so that

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

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

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

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

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

and

$$\phi_\ell = \phi_i - \phi_i'\left(\frac{h}{2}\right) + \frac{1}{2}\,\phi_i''\left(\frac{h}{2}\right)^2 - \frac{1}{6}\,\phi_i'''\left(\frac{h}{2}\right)^3 + \dots \tag{26}$$

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

$$\frac{\phi_r'' - \phi_\ell''}{h} = \phi_i''' + \frac{1}{24}\,\phi_i^{(\mathrm{v})}\,h^2 + \frac{1}{1920}\,\phi_i^{(\mathrm{vii})}\,h^4 + \dots \tag{27}$$

giving

$$\frac{\left(\dfrac{\phi_{i+1} + \phi_i}{2}\right) - \left(\dfrac{\phi_i + \phi_{i-1}}{2}\right)}{h} = \frac{(\phi_r - \phi_\ell)}{h} + \frac{1}{8}\,\phi_i'''\,h^2 + \frac{1}{128}\,\phi_i^{(\mathrm{v})}\,h^4 + \dots \tag{28}$$

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

$$(\mathrm{T.E.})_{\mathrm{FD}} = \frac{1}{6}\,\phi_i'''\,h^2 + \frac{1}{120}\,\phi_i^{(\mathrm{v})}\,h^4 + \dots \tag{29}$$

whereas

$$(\mathrm{T.E.})_{\mathrm{FV}} = \frac{1}{8}\,\phi_i'''\,h^2 + \frac{1}{128}\,\phi_i^{(\mathrm{v})}\,h^4 + \dots \tag{30}$$

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

$$(\mathrm{T.E.})_{\mathrm{FD}} - (\mathrm{T.E.})_{\mathrm{FV}} = \frac{1}{24}\,\phi_i'''\,h^2 + \frac{1}{1920}\,\phi_i^{(\mathrm{v})}\,h^4 + \dots \tag{31}$$

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 $(\phi_r - \phi_\ell)/h$. In fact, referring to Equations (25) and (26), continued through fifth-order, one finds that, irrespective of the numerical scheme,

$$\boxed{\frac{(\phi_r - \phi_\ell)}{h} = \left(\frac{\partial\phi}{\partial x}\right)_i + \frac{1}{24}\phi_i''' h^2 + \frac{1}{1920}\phi_i^{(v)} h^4 + \ldots} \tag{32}$$

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

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

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

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

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

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

and

$$(\phi_\ell)_{\text{model}} = \phi_{i-1} = \phi_\ell - \phi_\ell'\left(\frac{h}{2}\right) + \ldots \tag{36}$$

And this gives

$$\frac{(\phi_r - \phi_\ell)_{\text{model}}}{h} = \frac{(\phi_r - \phi_\ell)}{h} - \frac{1}{2}\left(\frac{\phi_r' - \phi_\ell'}{h}\right) h + \ldots \tag{37}$$

But, from Equations (17)-(20),

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

and

$$\phi_\ell' = \frac{(\phi_i - \phi_{i-1})}{h} - \frac{1}{24}\phi_\ell''' h^2 + \ldots \tag{39}$$

so that

$$\frac{\phi_r' - \phi_\ell'}{h} = \frac{(\phi_{i+1} - 2\phi_i + \phi_{i-1})}{h^2} - \frac{1}{24}\frac{(\phi_r''' - \phi_\ell''')}{h} h^2 + \ldots \tag{40}$$

and the second central-difference can be written

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

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

$$\frac{(\phi_r - \phi_\ell)_{\text{model}}}{h} = \frac{(\phi_r - \phi_\ell)}{h} - \frac{1}{2}\phi_i'' h + \ldots \tag{42}$$

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-biassed parabola through i, $(i-1)$, and $(i-2)$, the corresponding first-derivative at i is

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

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

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

$$\frac{\left(\frac{3}{2}\phi_i - \frac{1}{2}\phi_{i-1}\right) - \left(\frac{3}{2}\phi_{i-1} - \frac{1}{2}\phi_{i-2}\right)}{h} = \frac{(\phi_r - \phi_l)}{h} - \frac{3}{8}\phi_i''' h^2 + \frac{1}{4}\phi_i^{(iv)} h^3 + \ldots \tag{45}$$

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

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

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

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

and

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

But this gives

$$\frac{(\phi_r - \phi_\ell)_{\text{model}}}{h} = \frac{(\phi_r - \phi_\ell)}{h} - \tfrac{1}{24}\,\phi_i''' h^2 + \tfrac{1}{12}\,\phi_i^{(\text{iv})} h^3 + \ldots \tag{50}$$

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

In order 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 $u > 0$)

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

and

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

giving

$$\frac{(\phi_r - \phi_\ell)_{\text{model}}}{h} = \frac{\phi_r - \phi_\ell}{h} + \tfrac{1}{16}\,\phi_i^{(\text{iv})} h^3 - \tfrac{3}{128}\,\phi_i^{(\text{v})} h^4 + \ldots \tag{53}$$

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

$$\frac{1}{2}\left[(\phi_{i+2} - 3\phi_{i+1} + 3\phi_i - \phi_{i-1}) + (\phi_{i+1} - 3\phi_i + 3\phi_{i-1} - \phi_{i-2})\right]$$
$$= \frac{1}{2}(\phi_{i+2} - 2\phi_{i+1} + 2\phi_{i-1} - \phi_{i-2}) \tag{54}$$

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,

$$\frac{1}{2}\left[(\phi_{i+2} - 2\phi_{i+1} + \phi_i) + (\phi_{i+1} - 2\phi_i + \phi_{i-1})\right] = \frac{1}{2}(\phi_{i+2} - \phi_{i+1} - \phi_i + \phi_{i-1}) \tag{56}$$

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 $(\text{T.E.})_{\text{FD}}$, 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,

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

and then computes the control-volume cell average

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

the result is

$$\boxed{\bar{\phi}_i = \phi_i + \frac{1}{24}\phi_i'' h^2 + \frac{1}{1920}\phi_i^{(iv)} h^4 + \ldots} \tag{61}$$

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 thirteen years ago[1].

REFERENCE

1. B.P. Leonard, ''A Stable and Accurate Convective Modelling Procedure Based on Quadratic Upstream Interpolation,'' *Computer Methods in Applied Mechanics and Engineering*, **19**, 59-98 (1979).

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Judging by errors in the computational-fluid-dynamics literature in recent years, it is not generally well understood that (above first-order) there are 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.

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