reasonable line is to suggest that the face values between, for example, cell 4 and cell 5 are dependent only upon cell values from cell 4 or cells further upstream. Schemes that let face values be dependent only on upstream conditions are called *upwind schemes.* We will now examine two of these schemes closer.

First-order upwind

The idea behind the first-order upwind scheme is to have physical reliability for convective flows simply by letting the face value between two cells be equal to the value for the nearest upstream cell, i.e.

$$\begin{aligned}\phi_\mathrm{w} &= \phi_\mathrm{W},\\ \phi_\mathrm{e} &= \phi_\mathrm{P},\end{aligned} \tag{3.25}$$

or, for negative velocities,

$$\begin{aligned}\phi_\mathrm{w} &= \phi_\mathrm{P},\\ \phi_\mathrm{e} &= \phi_\mathrm{E}.\end{aligned} \tag{3.26}$$

The gradients are still estimated using Eq. (3.14).

If we return to our previous examples and use the first-order upwind scheme instead of the central-differencing scheme, we can rewrite Eq. (3.15) as

$$[(\rho U\phi_\mathrm{P}) - (\rho U\phi_\mathrm{W})] = \left[\left(\Gamma\frac{\phi_\mathrm{E}-\phi_\mathrm{P}}{x_\mathrm{E}-x_\mathrm{P}}\right) - \left(\Gamma\frac{\phi_\mathrm{P}-\phi_\mathrm{W}}{x_\mathrm{P}-x_\mathrm{W}}\right)\right]. \tag{3.27}$$

The physical meaning of the terms in the equation is the same as before; the difference in convective transport of ϕ is balanced out by the difference in diffusion. The only difference from Eq. (3.15) is that face values of ϕ have been expressed using the first-order upwind scheme instead of the central-differencing scheme. If we write Eq. (3.27) in the same form as Eq. (3.18), we get

$$\begin{aligned}a_\mathrm{E} &= \frac{\Gamma}{x_\mathrm{E}-x_\mathrm{P}},\\ a_\mathrm{W} &= \frac{\Gamma}{x_\mathrm{P}-x_\mathrm{W}} + \rho U,\\ a_\mathrm{P} &= \rho U + \frac{\Gamma}{x_\mathrm{E}-x_\mathrm{P}} + \frac{\Gamma}{x_\mathrm{P}-x_\mathrm{W}}.\end{aligned} \tag{3.28}$$

Then, 40 iterations with the GSA will yield the following values for the cells: $\phi_1 = 10.0004$, $\phi_2 = 10.0003$, $\phi_3 = 10.0003$, $\phi_4 = 10.0007$, $\phi_5 = 10.0034$, $\phi_6 = 10.0199$, $\phi_7 = 10.1191$, $\phi_8 = 10.7143$, $\phi_9 = 14.2858$ and $\phi_{10} = 35.7143$.

The results are as expected; the high flow rate makes the western boundary more dominant. Almost all cells in the domain, except the most eastern, have much the same value of ϕ of approximately 10. Again, this seems reasonable.

From Eq. (3.28) it follows that the first-order upwind scheme is bounded. It also fulfils the requirement of transportiveness since care is taken regarding the direction of the flow, cf. Eqs. (3.25) and (3.26). However, it also overestimates the transport of entities in the flow direction. This gives rise to so-called *numerical diffusion*.

Second-order upwind

To improve accuracy – we will discuss accuracy in more detail later – there is an upwind scheme that predicts the face values using information from two upwind cells. To estimate the eastern-face value, the scheme assumes that the gradient between the present cell and the eastern face is the same as that between the western cell and the present cell. In mathematical terms,

$$\frac{\phi_\mathrm{e}-\phi_\mathrm{P}}{x_\mathrm{e}-x_\mathrm{P}}=\frac{\phi_\mathrm{P}-\phi_\mathrm{W}}{x_\mathrm{P}-x_\mathrm{W}}\rightarrow\phi_\mathrm{e}=\frac{(\phi_\mathrm{P}-\phi_\mathrm{W})(x_\mathrm{e}-x_\mathrm{P})}{x_\mathrm{P}-x_\mathrm{W}}+\phi_\mathrm{P}. \tag{3.29}$$

For an equidistant grid, Eq. (3.29) gives that

$$\phi_\mathrm{e}=1.5\phi_\mathrm{P}-0.5\phi_\mathrm{W}. \tag{3.30}$$

A major drawback with the second-order upwind scheme is that it is *unbounded*. To avoid the numerical problems that often arise as a result of unbounded schemes, some *bounded* second-order schemes have been developed, e.g. the van Leer scheme. The definitions will be stated here.

The van Leer scheme

If $|\phi_\mathrm{E}-2\phi_\mathrm{P}+\phi_\mathrm{W}|\le|\phi_\mathrm{E}-\phi_\mathrm{W}|$, the value of ϕ at the eastern face is (cf. Eq. (3.29))

$$\phi_\mathrm{e}=\phi_\mathrm{P}+\frac{(\phi_\mathrm{E}-\phi_\mathrm{P})(\phi_\mathrm{P}-\phi_\mathrm{W})}{\phi_\mathrm{E}-\phi_\mathrm{W}}. \tag{3.31}$$

Otherwise (cf. Eq. (3.25)),

$$\phi_\mathrm{e}=\phi_\mathrm{P}. \tag{3.32}$$

The velocity is assumed to be positive. The van Leer scheme implements the unbounded second-order upwind scheme, Eq. (3.31), if the gradient is ‘smooth’, i.e. the second derivative of ϕ is ‘small’. Otherwise, the first-order upwind scheme, Eq. (3.32), is used.

3.8.4 Taylor expansions

Before proceeding, a short mathematical review of Taylor expansions will be given.

Taylor's theorem for a 1D expansion of a real function $f(x)$ about a point $x=x_0$ is given without a proof:

$$\begin{aligned}f(x)&=f(x_0)+(x-x_0)f'(x_0)+\frac{(x-x_0)^2}{2!}f''(x_0)+\cdots\\&\quad+\frac{(x-x_0)^n}{n!}f^{(n)}(x_0)+\int_{x_0}^{x}\frac{(x-u)^n}{n!}f^{(n+1)}(u)\mathrm{d}u.\end{aligned} \tag{3.33}$$

The last term in Eq. (3.33) is called the *Lagrange remainder*. Taylor's theorem, except for the Lagrange remainder, was devised by the English mathematician Brook Taylor in 1712 and published in *Methodus in crementorum directa et inversa* in 1715. The more terms are included in the series, the more accurate the estimation will be. Taylor expansions will be used when discussing accuracy.

3.8.5 Accuracy

Two different types of discretization schemes have been presented, the central-differencing scheme and the upwind schemes, one that fulfils the requirement of transportiveness and one that does not. The last section concluded that for problems with strong convection the central-differencing scheme failed. The first-order upwind scheme was then used instead. On the other hand, the first-order upwind scheme used only one cell to estimate the face value, compared with two cells for the central-differencing scheme, and thus we should expect the first-order upwind scheme to be less *accurate* than the central-differencing scheme. Generally, the more information is used, the better the estimation. Accuracy can be quantified in several ways.

For the central-differencing scheme, we have

$$\begin{aligned}\phi_\mathrm{w} &= \frac{\phi_\mathrm{W}+\phi_\mathrm{P}}{2},\\ \phi_\mathrm{e} &= \frac{\phi_\mathrm{P}+\phi_\mathrm{E}}{2}\end{aligned} \tag{3.13}$$

and

$$\begin{aligned}\left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_\mathrm{w} &= \frac{\phi_\mathrm{P}-\phi_\mathrm{W}}{x_\mathrm{P}-x_\mathrm{W}},\\ \left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_\mathrm{e} &= \frac{\phi_\mathrm{E}-\phi_\mathrm{P}}{x_\mathrm{E}-x_\mathrm{P}}.\end{aligned} \tag{3.14}$$

If it is assumed that the grid is equidistant (this has been the case in all our examples so far), the *grid spacing* can be defined as $\Delta x = x_\mathrm{P} - x_\mathrm{W} = x_\mathrm{E} - x_\mathrm{P}$. If a Taylor expansion of ϕ_E and ϕ_P is made about x_e, the following result is reached:

$$\begin{aligned}\phi_\mathrm{E} = \phi_\mathrm{e} &+ (\Delta x/2)\left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_\mathrm{e} + \frac{(\Delta x/2)^2}{2}\left(\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}\right)_\mathrm{e} + \frac{(\Delta x/2)^3}{6}\left(\frac{\mathrm{d}^3\phi}{\mathrm{d}x^3}\right)_\mathrm{e}\\ &+ \frac{(\Delta x/2)^4}{24}\left(\frac{\mathrm{d}^4\phi}{\mathrm{d}x^4}\right)_\mathrm{e} + O\left[(\Delta x)^5\right],\end{aligned} \tag{3.34}$$

$$\begin{aligned}\phi_\mathrm{P} = \phi_\mathrm{e} &- (\Delta x/2)\left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_\mathrm{e} + \frac{(\Delta x/2)^2}{2}\left(\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}\right)_\mathrm{e} - \frac{(\Delta x/2)^3}{6}\left(\frac{\mathrm{d}^3\phi}{\mathrm{d}x^3}\right)_\mathrm{e}\\ &+ \frac{(\Delta x/2)^4}{24}\left(\frac{\mathrm{d}^4\phi}{\mathrm{d}x^4}\right)_\mathrm{e} + O\left[(\Delta x)^5\right].\end{aligned} \tag{3.35}$$

Here, $O[(\Delta x)^n]$ is the *truncation error*. Next, Eqs. (3.34) and (3.35) are inserted into the right-hand side of the second equation in Eqs. (3.13) and (3.14), which results in

$$\frac{\phi_\mathrm{P}+\phi_\mathrm{E}}{2} = \phi_\mathrm{e} + \frac{(\Delta x)^2}{8}\left(\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}\right)_\mathrm{e} + \frac{(\Delta x)^4}{384}\left(\frac{\mathrm{d}^4\phi}{\mathrm{d}x^4}\right) + O\left[(\Delta x)^6\right], \tag{3.36}$$

$$\frac{\phi_\mathrm{E}-\phi_\mathrm{P}}{\Delta x} = \left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_\mathrm{e} + \frac{(\Delta x)^2}{24}\left(\frac{\mathrm{d}^3\phi}{\mathrm{d}x^3}\right)_\mathrm{e} + O\left[(\Delta x)^5\right]. \tag{3.37}$$

According to Eqs. (3.13) and (3.14), these expressions should be equal to the face value of ϕ and the gradient of ϕ at the eastern face, respectively, *assuming that central differencing is used*. Thus, since the second-order derivative $\mathrm{d}^2\phi/\mathrm{d}x^2$ is unknown,

$$\phi_\mathrm{e} = \phi_\mathrm{e}^{\mathrm{CD}} + O\left[(\Delta x)^2\right] \tag{3.38}$$

and

$$\left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_\mathrm{e} = \left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_\mathrm{e}^{\mathrm{CD}} + O\left[(\Delta x)^2\right]. \tag{3.39}$$

Before we comment on the results, we repeat the same procedure for the first-order upwind scheme. Since the face gradient is predicted in the same way as with central differencing, the face-value estimation, i.e. Eq. (3.25), must be examined. According to this relation, the face value of the eastern face is simply equal to the cell value in the present cell. A Taylor expansion of ϕ about x_P gives

$$\phi_\mathrm{e} = \phi_\mathrm{P} + (\Delta x/2)\left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_\mathrm{P} + \frac{(\Delta x/2)^2}{2}\left(\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}\right)_\mathrm{P} + O\left[(\Delta x)^3\right]. \tag{3.40}$$

Here, the first-order derivative is unknown and the outcome is

$$\phi_\mathrm{e} = \phi_\mathrm{e}^{\mathrm{1u}} + O(\Delta x). \tag{3.41}$$

If Eqs. (3.38) and (3.41) are compared, it can be seen that, for a reduction of Δx, the face-value estimation seems to approach the 'true' value quicker in the case with the central-differencing scheme. In other words, this means that, if the grid is made denser, i.e. more cells are introduced, the error in the central-differencing scheme will be reduced more quickly than in the case with the first-order upwind scheme. The lowest order of the grid spacing in the central-differencing scheme is 2, hence the central-differencing scheme is referred to as *second-order accurate*. For the first-order upwind scheme, the corresponding number is 1; hence this scheme is referred to as *first-order accurate*.

Higher-order schemes are more accurate but this can be at the expense of numerical stability. When stability is problematic it is recommended that one start with a simple first-order upwind scheme and change to a higher-order scheme after some iterations. Going to higher order is always necessary in order to minimize numerical diffusion when the grids are not aligned with the flow.

3.8.6 The hybrid scheme

An attempt to combine the positive properties of both the central-differencing scheme and the first-order upwind scheme has been proposed. This scheme is called the *hybrid differencing scheme*. This scheme implements the upwind scheme at faces where the criterion in Eq. (3.24) is fulfilled, and uses central differencing elsewhere. Thus, this scheme takes advantage of both the high accuracy of the central-differencing scheme and the more physical properties in terms of boundedness and transportiveness of the upwind scheme.

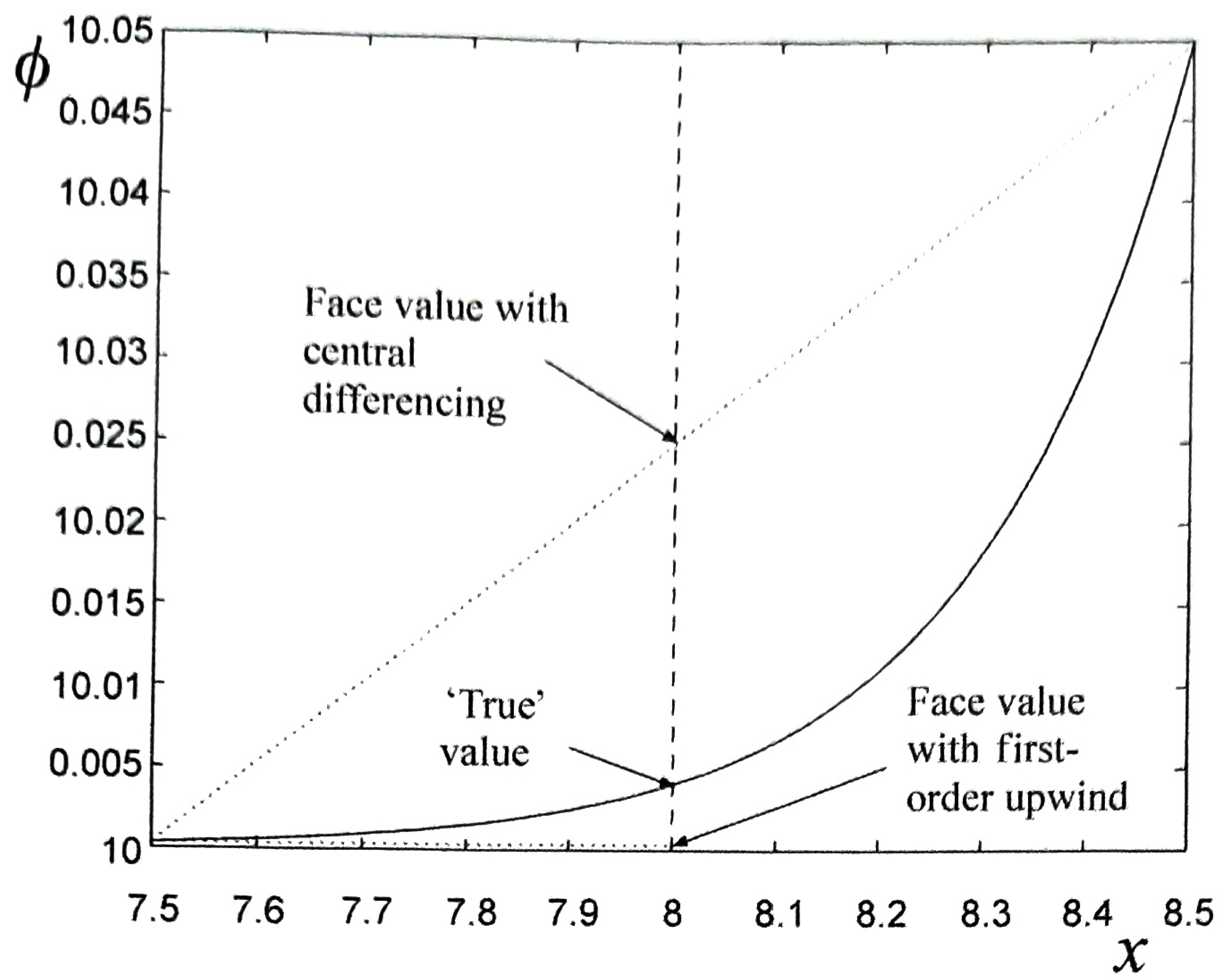

Figure 3.10 Face-value approximations of the face between cells 8 and 9 with central differencing and first-order upwind, respectively. The analytical ('true') solution which, in this specific case, corresponds to the power-law prediction has been added for comparison. $U = 5$ cm s^{-1}.

3.8.7 The power-law scheme

A more accurate scheme is the *power-law scheme*. Briefly, the face value of ϕ is estimated by solving a convection–diffusion equation (cf. Eq. (3.1)),

$$\rho \frac{\mathrm{d}(U\phi)}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\Gamma \frac{\mathrm{d}\phi}{\mathrm{d}x}\right). \tag{3.42}$$

Equation (3.42) has the following solution, assuming constant fluid and flow properties:

$$\frac{\phi(x) - \phi_0}{\phi_{\Delta x} - \phi_0} = \frac{\exp(\rho U x/\Gamma) - 1}{\exp(\rho U \, \Delta x/\Gamma) - 1}, \tag{3.43}$$

where the indices 0 and Δx represent two neighbouring cells. If the grid spacing is equidistant, the face is situated at $x = 0.5$. The face value can now be estimated using Eq. (3.43). If the parameters from the previous examples are used, the plot of $\phi(x)$ against x will clearly show that for $U = 5$ cm s^{-1} the face value is almost exactly the same as for the upstream cell; see Figure 3.10. The central-differencing scheme makes a bad estimation of the face value. This was the reason why the upwind scheme was chosen in Example 3.

3.8.8 The QUICK scheme

Numerous successful attempts have been made to create numerical schemes with higher accuracy than second order. One of them will very briefly be discussed, namely QUICK (Quadratic Upstream Interpolation for Convective Kinetics). QUICK combines the strengths of both the upwind schemes and of the central differencing; it uses three-point upstream quadratic interpolation to estimate the face values. For the western and eastern faces, respectively,

$$\phi_{\mathrm{w}} = \frac{6}{8}\phi_{\mathrm{W}} + \frac{3}{8}\phi_{\mathrm{P}} - \frac{1}{8}\phi_{\mathrm{WW}}, \tag{3.44}$$

$$\phi_{\mathrm{e}} = \frac{6}{8}\phi_{\mathrm{P}} + \frac{3}{8}\phi_{\mathrm{E}} - \frac{1}{8}\phi_{\mathrm{W}}. \tag{3.45}$$

It has been assumed here that the velocity is positive. A Taylor expansion of ϕ around the eastern face gives

$$\phi_{\mathrm{E}} = \phi_{\mathrm{e}} + (\Delta x/2)\left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_{\mathrm{e}} + \frac{(\Delta x/2)^2}{2}\left(\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}\right)_{\mathrm{e}} + O\left[(\Delta x)^3\right], \tag{3.34$'$}$$

$$\phi_{\mathrm{P}} = \phi_{\mathrm{e}} - (\Delta x/2)\left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_{\mathrm{e}} + \frac{(\Delta x/2)^2}{2}\left(\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}\right)_{\mathrm{e}} + O\left[(\Delta x)^3\right], \tag{3.35$'$}$$

$$\phi_{\mathrm{W}} = \phi_{\mathrm{e}} - (1.5\Delta x)\left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_{\mathrm{e}} + \frac{(1.5\Delta x)^2}{2}\left(\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}\right)_{\mathrm{e}} + O\left[(\Delta x)^3\right]. \tag{3.46}$$

On inserting Eqs. (3.34′), (3.35′) and (3.46) into Eq. (3.45), we get

$$\phi_{\mathrm{e}} = \phi_{\mathrm{e}}^{\mathrm{QUICK}} + O\left[(\Delta x)^3\right]. \tag{3.47}$$

Thus, the QUICK scheme is *third-order accurate*. Further, it can be shown that it is *unbounded* but fulfils the *transportiveness* criterion. The use of QUICK is restricted to hexahedral meshes.

3.8.9 More advanced discretization schemes

The discretization schemes mentioned previously are only a few among the many available. In most commercial CFD codes there are many variations of schemes, and it is not our intention to provide a complete list in Table 3.1. However, two more will be mentioned here without going into too much detail.

- MUSCL (Monotone Upstream-centred Schemes for Conservation Laws). The MUSCL scheme shows a similar degree of accuracy to QUICK, but is not limited to hexahedral meshes.
- HRIC (High-Resolution Interface Capturing). The HRIC scheme is primarily used in multiphase flows when tracking the interface between the phases. HRIC has proven to be more accurate than QUICK for VOF simulations (see Chapter 6).

For all of the discretization schemes that have been presented here, the error tends to zero as the grid spacing is reduced infinitely. Schemes that uphold this property are said to be *consistent*. It should also be mentioned that the definitions of some of the discretization schemes presented here seem to differ in the literature.