$$\left[\frac{\partial(\rho u\phi)}{\partial x}\right]_i \approx \rho u \frac{\phi_{i+1}-\phi_{i-1}}{x_{i+1}-x_{i-1}} . \tag{3.68}$$

The CDS contributions to the coefficients of Eq. (3.64) are:

$$A_{\mathrm{E}}^{\mathrm{c}} = \frac{\rho u}{x_{i+1}-x_{i-1}} ; \qquad A_{\mathrm{W}}^{\mathrm{c}} = -\frac{\rho u}{x_{i+1}-x_{i-1}} ;$$

$$A_{\mathrm{P}}^{\mathrm{c}} = -(A_{\mathrm{E}}^{\mathrm{c}} + A_{\mathrm{W}}^{\mathrm{c}}) = 0 .$$

The total coefficients are the sums of the convection and diffusion contributions, A^{c} and A^{d}.

The values of ϕ at boundary nodes are specified: $\phi_1 = \phi_0$ and $\phi_N = \phi_L$, where N is the number of nodes including the two at the boundaries. This means that, for the node at $i = 2$, the term $A_{\mathrm{W}}^2\phi_1$ can be calculated and added to Q_2, the right hand side, and we set the coefficient A_{W}^2 in that equation to zero. Analogously, we add the product $A_{\mathrm{E}}^{N-1}\phi_N$ for the node $i = N-1$ to Q_{N-1} and set the coefficient $A_{\mathrm{E}}^{N-1} = 0$.

The resulting tridiagonal system is easily solved. We shall only discuss the solutions here; the solver used to obtain them will be introduced in Chap. 5.

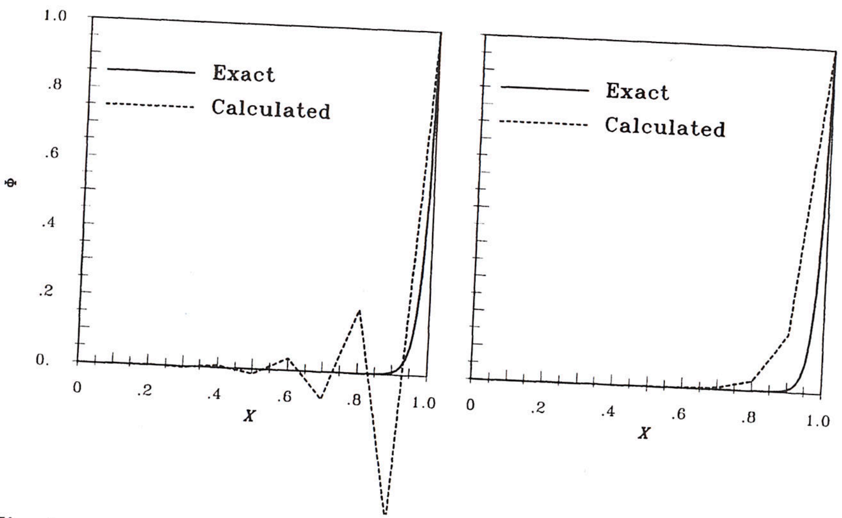

Fig. 3.8. Solution of the 1D convection/diffusion equation at Pe = 50 using CDS (left) and UDS (right) for convection terms and a uniform grid with 11 nodes

In order to demonstrate the false diffusion associated with UDS and the possibility of oscillations when using CDS, we shall consider the case with Pe = 50 ($L = 1.0$, $\rho = 1.0$, $u = 1.0$, $\Gamma = 0.02$, $\phi_0 = 0$ and $\phi_L = 1.0$). We start with results obtained using uniform grid with 11 nodes (10 equal subdivisions). The profiles of $\phi(x)$ obtained using CDS and UDS for convection and CDS for diffusion terms are shown in Fig. 3.8.

The UDS solution is obviously over-diffusive; it corresponds to the exact solution for Pe $\approx$ 18 (instead of 50). The false diffusion is stronger than the true diffusion! On the other hand, the CDS solution exhibits severe oscillations. The oscillations are due to the sudden change of gradient in ϕ at the last two points. The Peclet number based on mesh spacing (see Eq. (3.63)) is equal to 5 at every node.

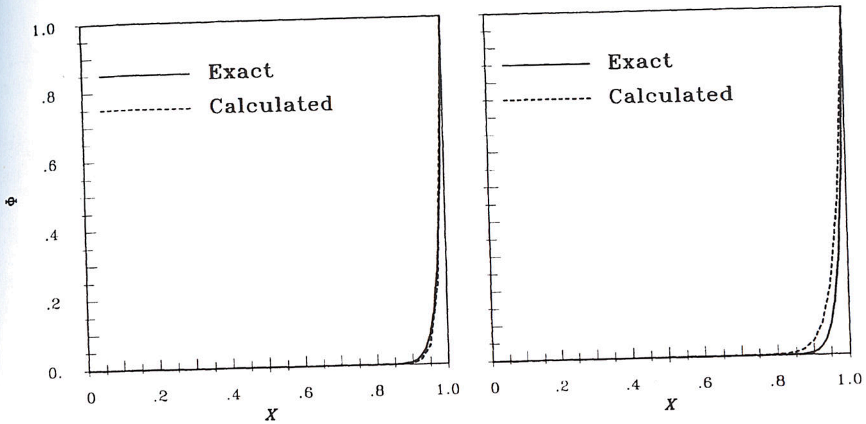

Fig. 3.9. Solution of the 1D convection/diffusion equation at Pe = 50 using CDS (left) and UDS (right) for convection terms and a uniform grid with 41 nodes

If the grid is refined, the CDS oscillations are reduced, but they are still present when 21 points are used. After the second refinement (41 grid nodes), the solution is oscillation-free and very accurate, see Fig. 3.9. The accuracy of the UDS solution has also been improved by grid refinement, but it is still substantially in error for $x > 0.8$.

The CDS oscillations depend on the value of the local Peclet number, $\mathrm{Pe} = \rho u \Delta x/\Gamma$. It can be shown that no oscillations occur if the local Peclet number is $\mathrm{Pe} \leq 2$ at every grid node (see Patankar, 1980). This is a sufficient, but not necessary condition for boundedness of CDS solution. The so-called *hybrid scheme* (Spalding, 1972) was designed to switch from CDS to UDS at any node at which $\mathrm{Pe} \geq 2$. This is too restrictive and reduces the accuracy. Oscillations appear only when the solution changes rapidly in a region of high local Peclet number.

In order to demonstrate this, we repeat the calculation using a non-uniform grid with 11 nodes. The smallest and the largest mesh spacings are $\Delta x_{\min} = x_N - x_{N-1} = 0.0125$ and $\Delta x_{\max} = x_2 - x_1 = 0.31$, corresponding to can be relaxed by using functions other than complex exponentials but any change in geometry or boundary conditions requires a considerable change in the method, making spectral methods relatively inflexible. For the problems to which they are ideally suited (for example, the simulation of turbulence in geometrically simple domains), they are unsurpassed.

3.10.2 Another View of Discretization Error

Spectral methods are as useful for providing another way of looking at truncation errors as they are as computational methods on their own. So long as we deal with periodic functions, the series (3.54) represents the function and we may approximate its derivative by any method we choose. In particular, we can use the exact spectral method of the example above or a finite difference approximation. Any of these methods can be applied term-by-term to the series so it is sufficient to consider differentiation of $\mathrm{e}^{\mathrm{i}kx}$. The exact result is $\mathrm{i}k\mathrm{e}^{\mathrm{i}kx}$. On the other hand, if we apply the central difference operator of Eq. (3.9) to this function we find:

$$\frac{\delta \mathrm{e}^{\mathrm{i}kx}}{\delta x} = \frac{\mathrm{e}^{\mathrm{i}k(x+\Delta x)} - \mathrm{e}^{\mathrm{i}k(x-\Delta x)}}{2\Delta x} = \mathrm{i}\,\frac{\sin(k\,\Delta x)}{\Delta x}\,\mathrm{e}^{\mathrm{i}kx} = \mathrm{i}k_{\mathrm{eff}}\,\mathrm{e}^{\mathrm{i}kx}\ , \tag{3.57}$$

where k_{eff} is called the *effective wavenumber* because using the finite difference approximation is equivalent to replacing the exact wavenumber k by k_{eff}. Similar expressions can be derived for other schemes; for example, the fourth order CDS, Eq. (3.14), leads to:

$$k_{\mathrm{eff}} = \frac{\sin(k\,\Delta x)}{3\Delta x}\,[4 - \cos(k\,\Delta x)]\ . \tag{3.58}$$

For low wavenumber (corresponding to smooth functions), the effective wavenumber of the CDS approximation can be expanded in a Taylor series:

$$k_{\mathrm{eff}} = \frac{\sin(k\,\Delta x)}{\Delta x} = k - \frac{k^3(\Delta x)^2}{6}\ , \tag{3.59}$$

which shows the second-order nature of the approximation for small k and small Δx. However, in any computation, wavenumbers up to $k_{\max} = \pi/\Delta x$ may be encountered. The magnitude of a given Fourier coefficient depends on the function whose derivatives are being approximated; smooth functions have small high wavenumber components but rapidly varying functions give Fourier coefficients that decrease slowly with wavenumber.

In Fig. 3.6 the effective wavenumbers of the second and fourth order CDS scheme, normalized by $k_{\max}$, are shown as functions of the normalized wavenumber $k^* = k/k_{\max}$. Both schemes give a poor approximation if the wavenumber is larger than half the maximum value. More wavenumbers are ... of small spacings, the function is

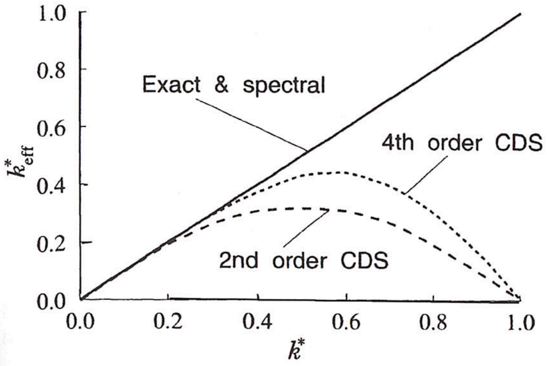

Fig. 3.6. Effective wavenumber for the second and fourth order CDS approximation of the first derivative, normalized by $k_{\max} = \pi/\Delta x$

smooth relative to the grid, only the small wavenumbers have large coefficients, and accurate results may be expected.

If we are solving a problem with a solution that is not very smooth, the order of the discretization method may no longer be a good indicator of its accuracy. One needs to be very careful about claims that a particular scheme is accurate because the method used is of high order. The result is accurate only if there are enough nodes per wavelength of a highest wavenumber in the solution.

Spectral methods yield an error that decreases more rapidly than any power of the grid size as the latter goes to zero. This is often cited as an advantage of the method. However, this behavior is obtained only when enough points are used (the definition of 'enough' depends on the function). For small numbers of grid points, spectral methods may actually yield larger errors than finite difference methods.

Finally, we note that the effective wavenumber of the upwind difference method is:

$$k_{\mathrm{eff}} = \frac{1 - \mathrm{e}^{-\mathrm{i}k\,\Delta x}}{\Delta x} \tag{3.60}$$

and is complex. This is an indication of the dissipative nature of this approximation.

3.11 Example

In this example we solve the steady 1D convection/diffusion equation with Dirichlet boundary conditions at both ends. The aim is to demonstrate the properties of the FD discretization technique for a simple problem which has an analytic solution.

The equation to be solved reads (see Eq. (1.28)):